Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 1

Title: Method and System for Data Analysis
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Inventors: Grinstein, et al.
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Fig. 2

Title: Method and System for Data Analysis
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Fig. 3

Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
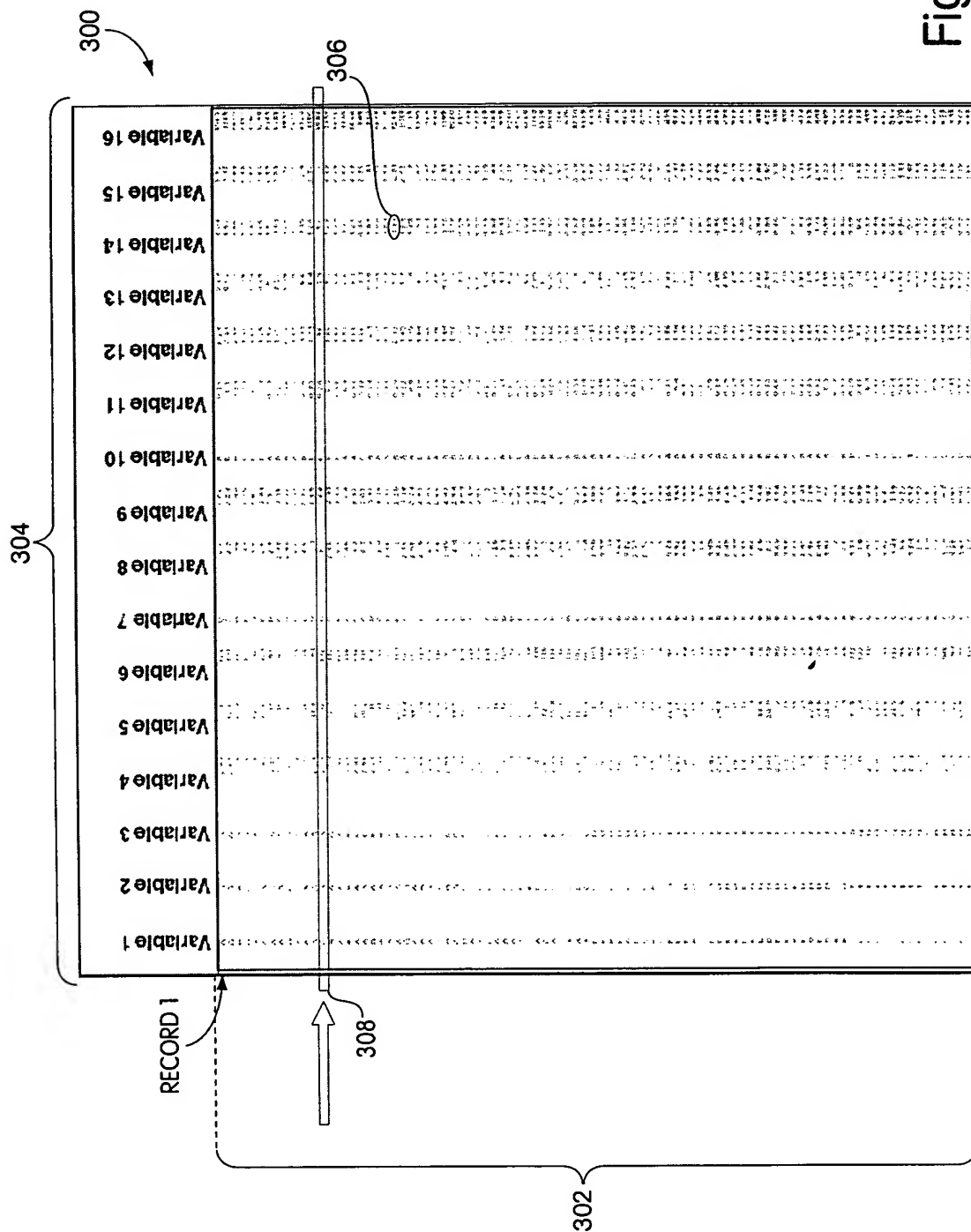Atty. Docket No.: ANVI-P01-001

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Fig. 4A

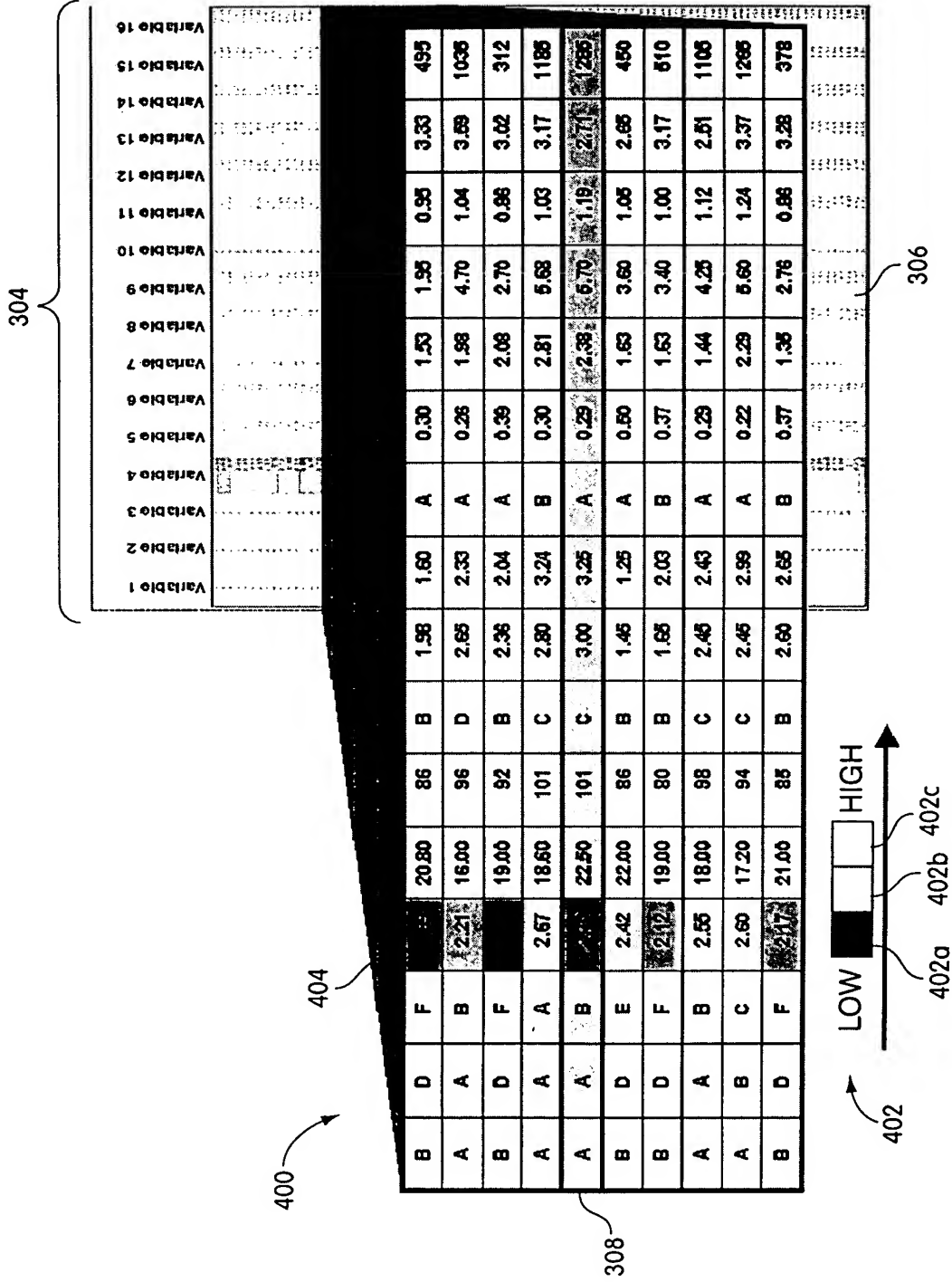**Fig. 4B**

LOW — HIGH
402a 402b 402c
402

400 406 308 304 306

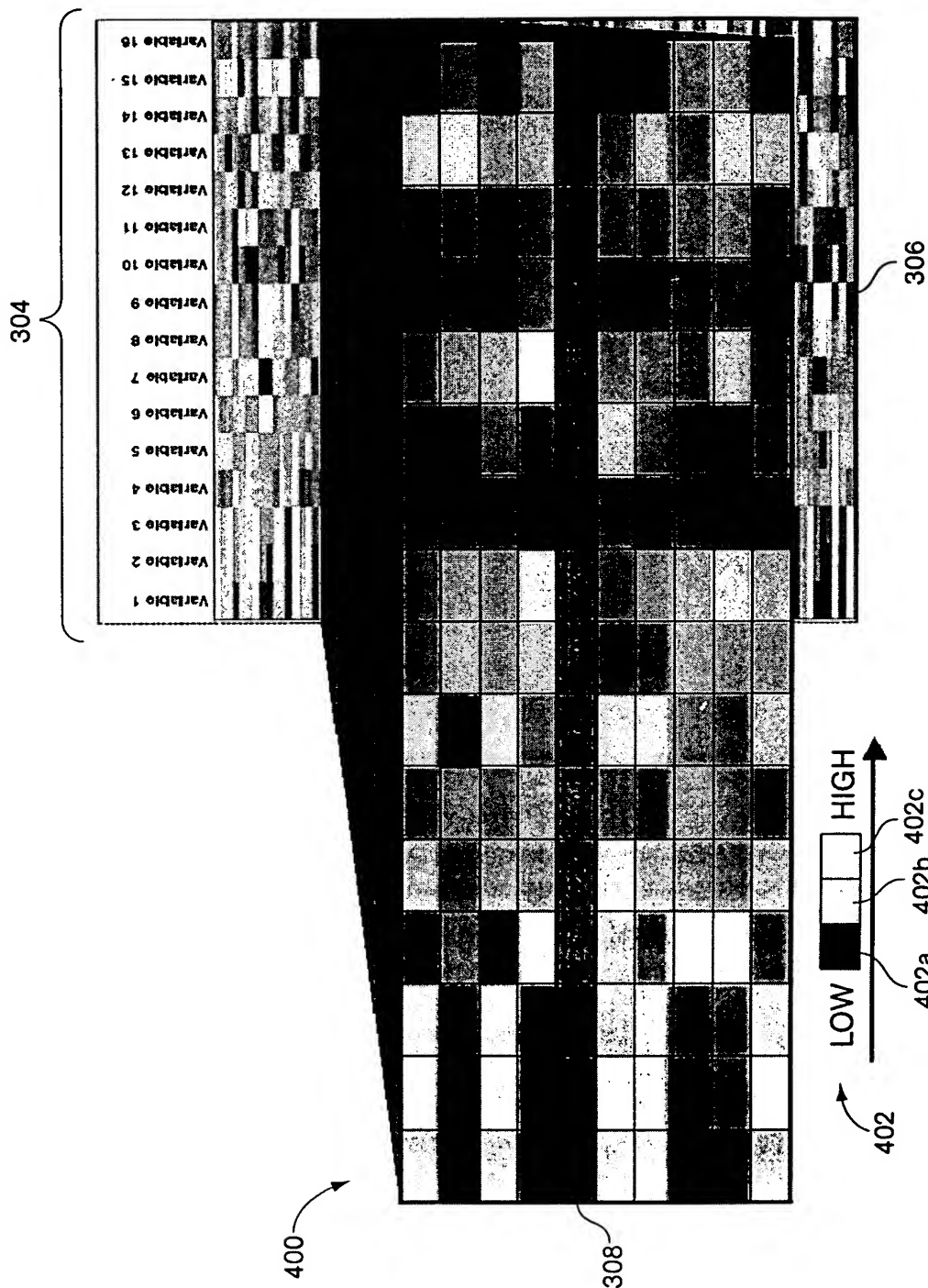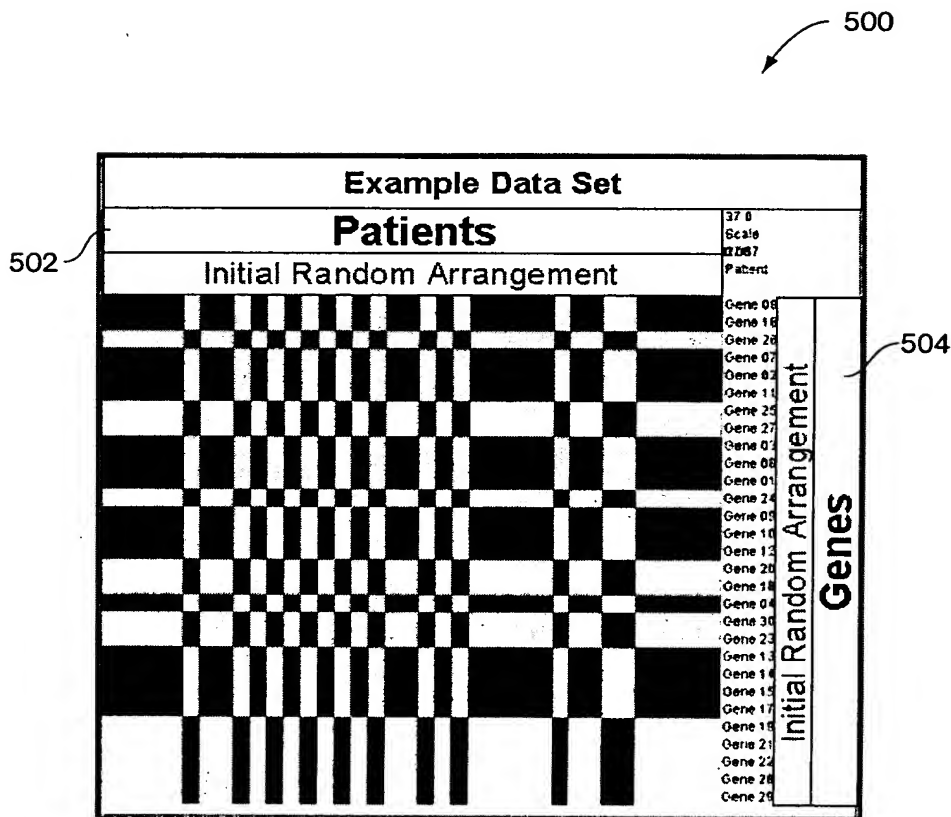|	Variable 1	Variable 2	Variable 3	Variable 4	Variable 5	Variable 6	Variable 7	Variable 8	Variable 9	Variable 10	Variable 11	Variable 12	Variable 13	Variable 14	Variable 15	Variable 16
B	D	F	1.99	20.80	86	B	1.98	1.60		A	0.30		1.53		1.95	0.95		3.33	495	
A		B	2.21	16.00	96	D	2.65	2.33		A	0.26		1.98		4.70	1.04		3.59	1035	
B	D	F	1.94	19.00	92	B	2.36	2.04		A	0.39		2.08		2.70	0.86		3.02	312	
A		A	2.57	18.60	101	C	2.80	3.24		B	0.30		2.81		5.68	1.03		3.17	1155	
A		B	2.70	22.50	101	C	3.00	3.25		A	0.29		2.38		5.70	1.19		2.74	1295	
B	D	E	2.42	22.00	86	B	1.45	1.25		A	0.50		1.63		3.60	1.05		2.65	460	
B	D	F	2.12	19.00	80	B	1.65	2.03		B	0.37		1.63		3.40	1.00		3.17	510	
A	C	B	2.55	18.00	98	C	2.45	2.43		A	0.29		1.44		4.25	1.12		2.51	1105	
A	CB	C	2.60	17.20	94	C	2.45	2.99		A	0.22		2.29		5.60	1.24		3.37	1265	
B	D	F	2.17	21.00	85	B	2.60	2.65		B	0.37		1.35		2.76	0.86		3.28	378	

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Fig. 4C

Title: Method and System for Data Analysis
Serial No.: 10/077,694
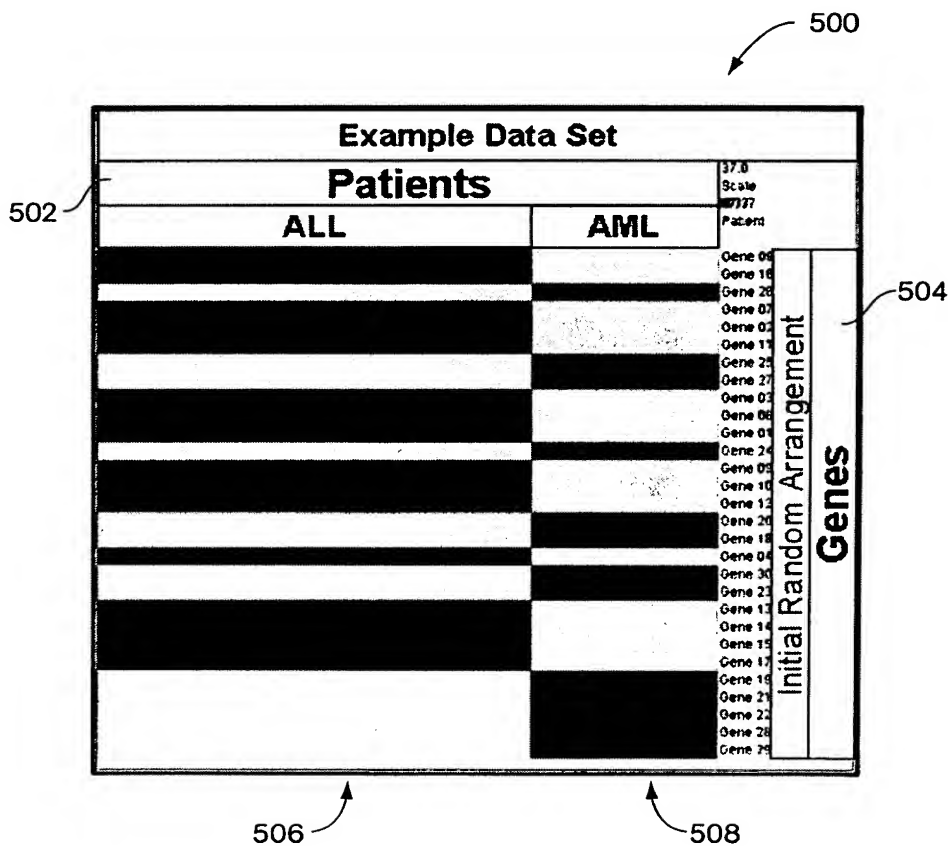Inventors: Grinstein, et al.
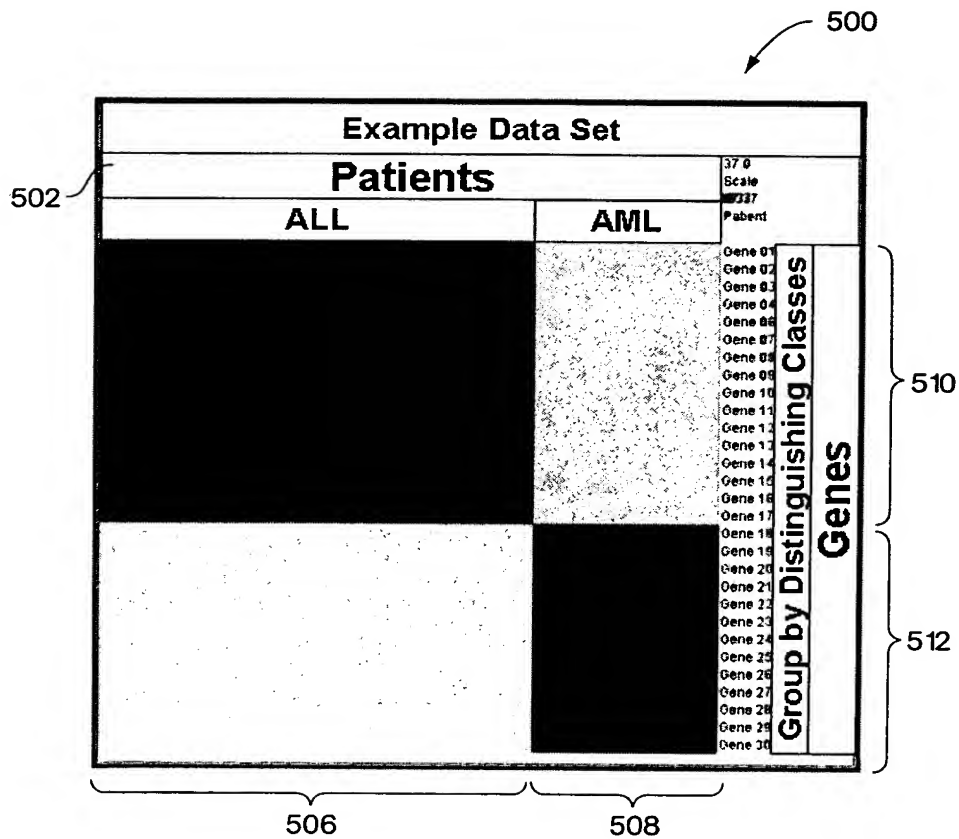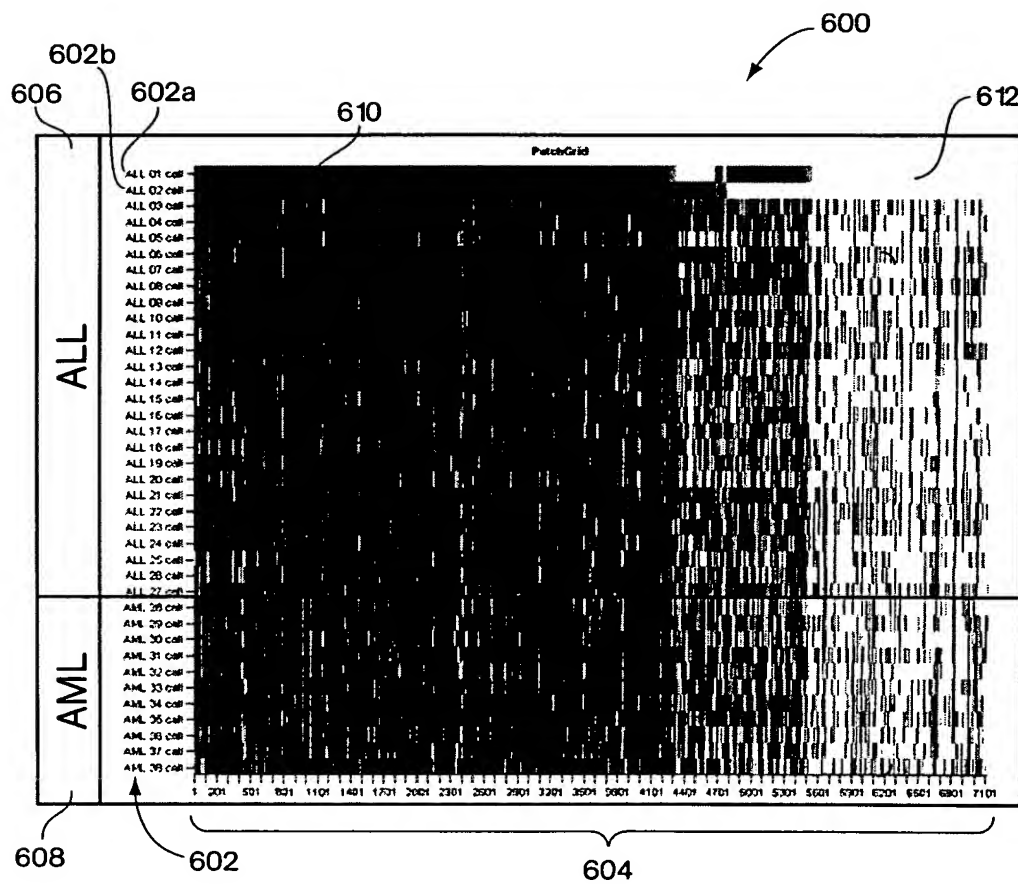Atty. Docket No.: ANVI-P01-001

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Fig. 4D

500

Example Data Set
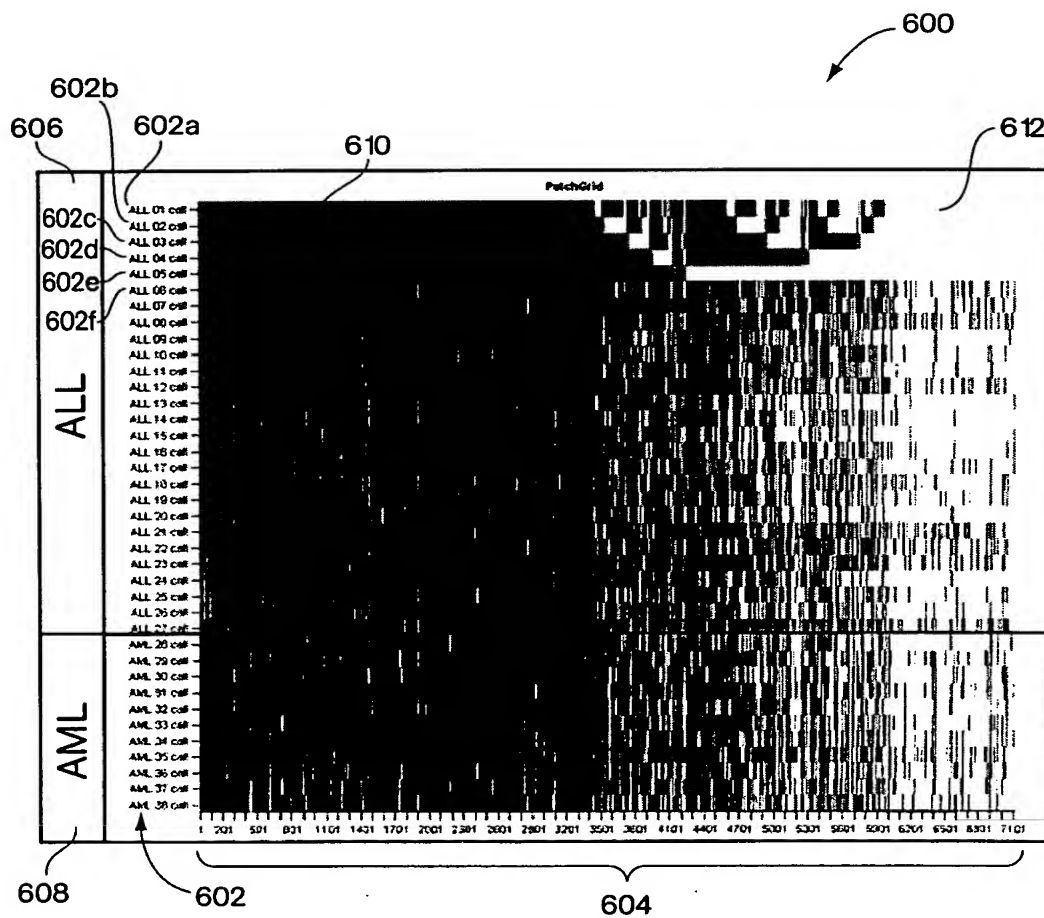
Patients

502

Initial Random Arrangement

504

Genes

Initial Random Arrangement

Fig. 5A

Fig. 5B

Title: Method and System for Data Analys[is]
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Inventors: Grinstein, et al.
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Example Data Set

Fig. 5C

Method and System for Data Analysis
Serial No.: 10/077,694
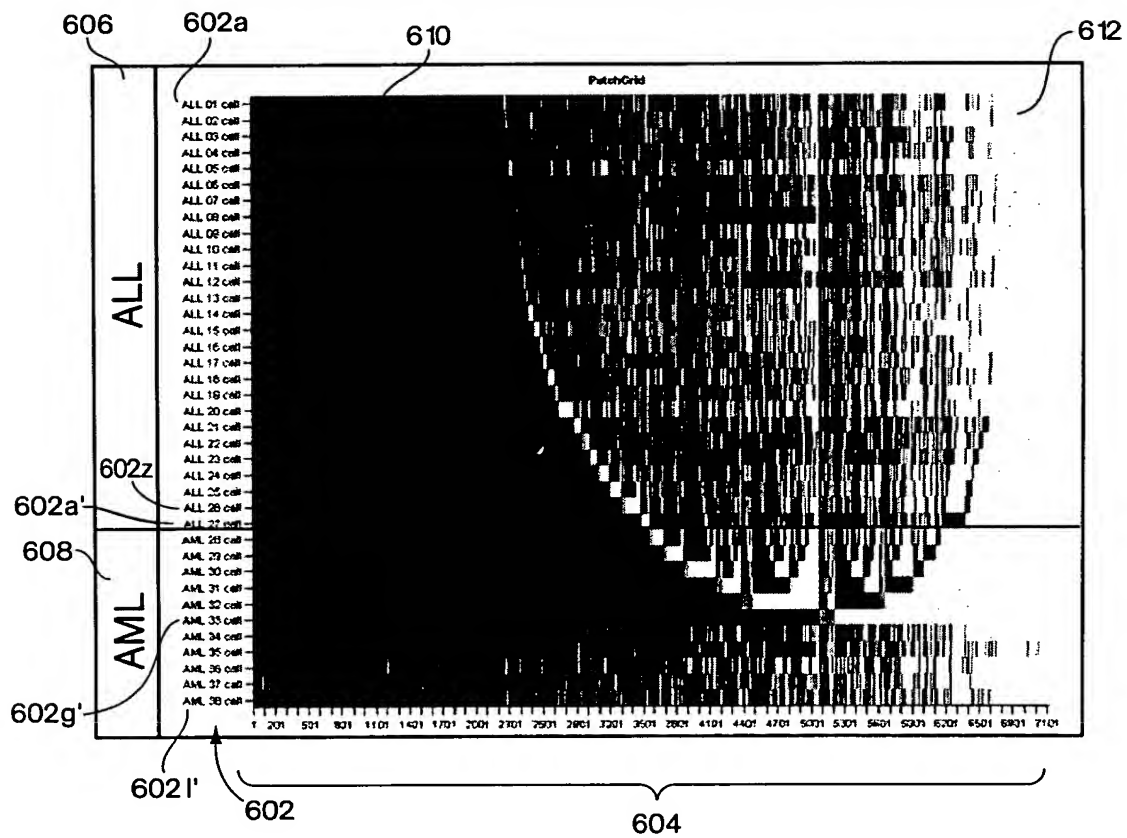Inventors: Grinstein, et al.
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Fig. 6A

Fig. 6B

Method and System for Data Analysis
Serial No.: 10/077,694
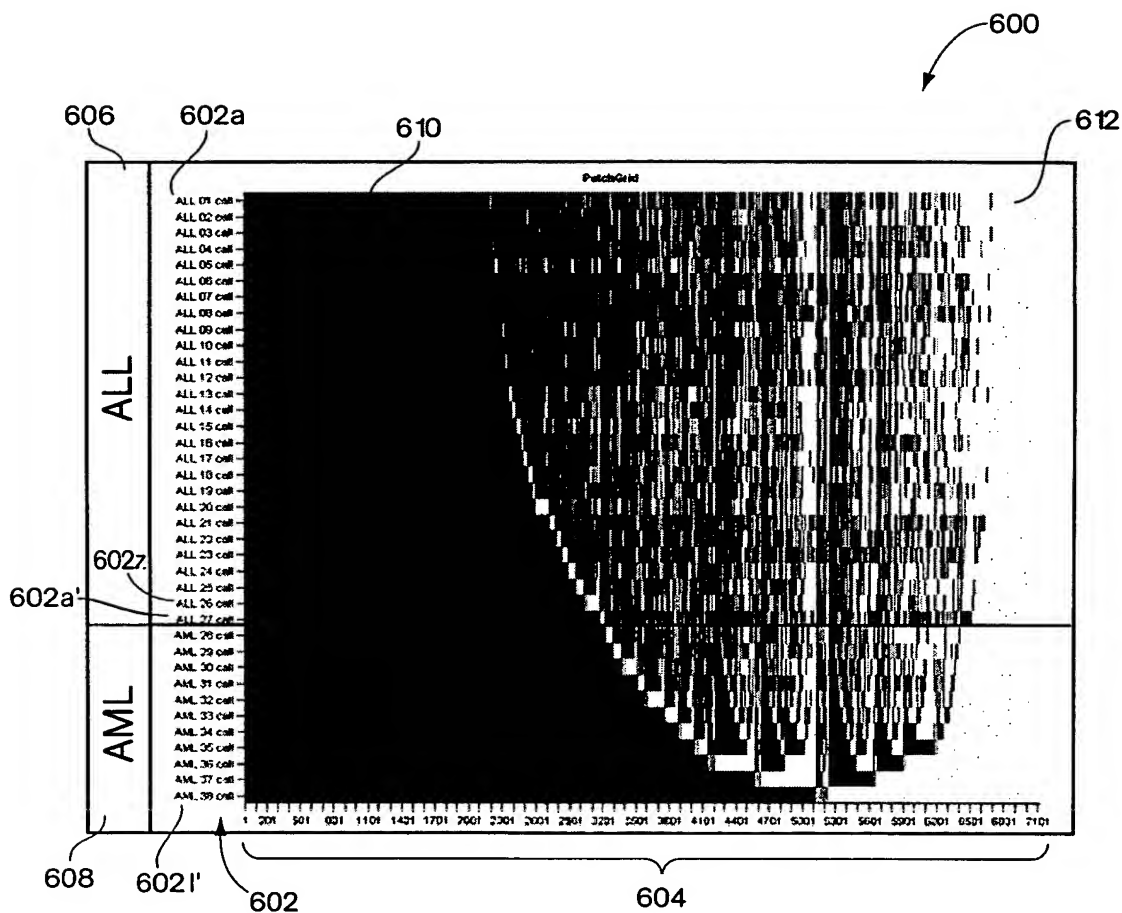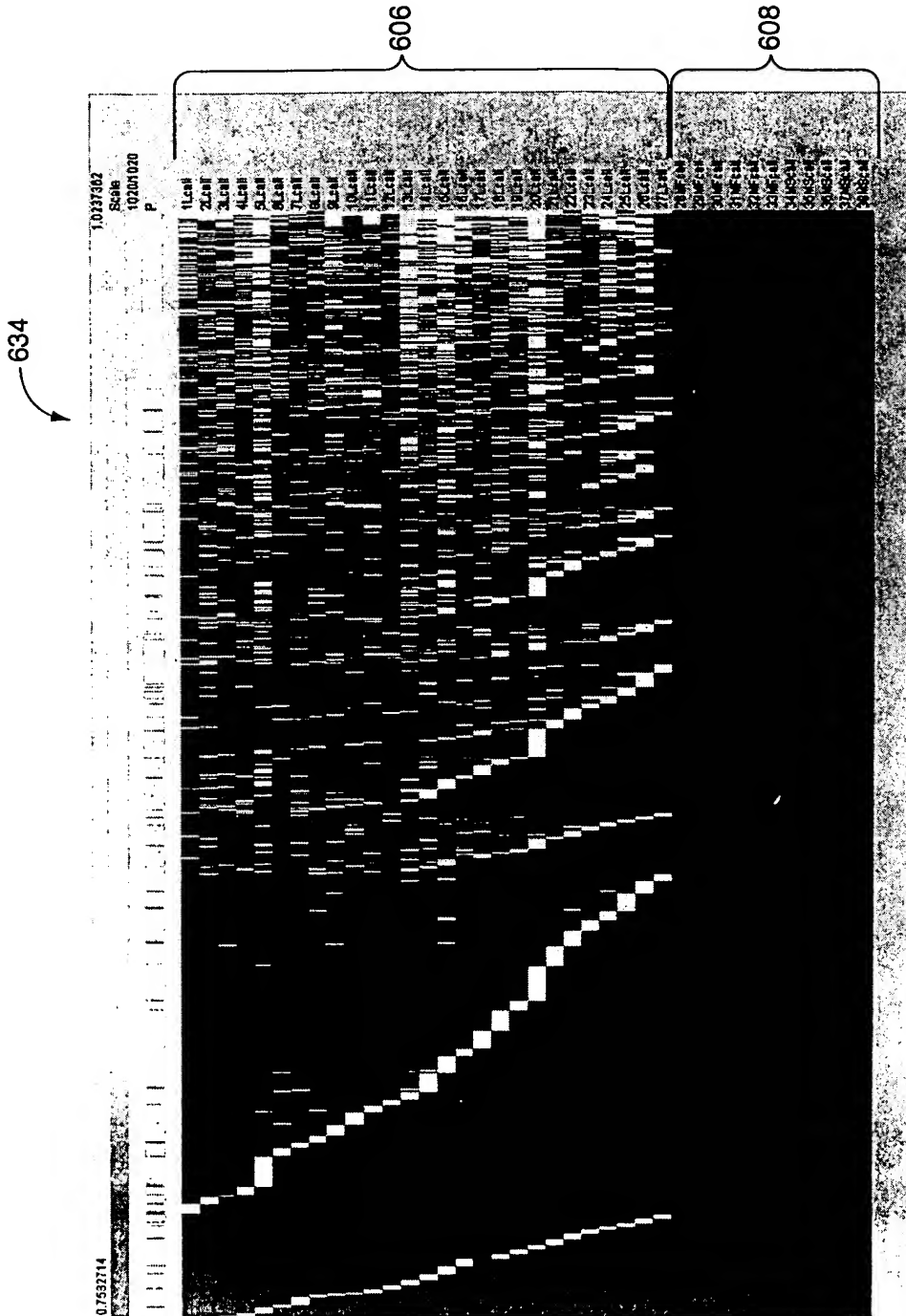Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 6C

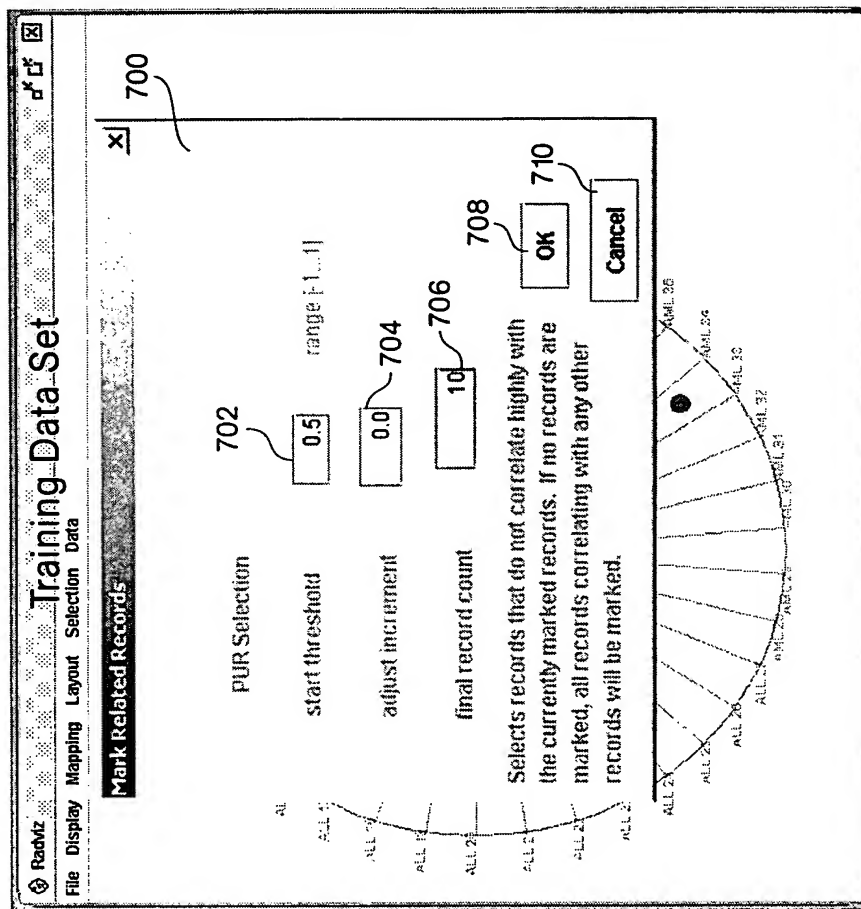Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

Fig. 6D

Title: Method and System for Data Anal...
...ial No.: 10/077,694
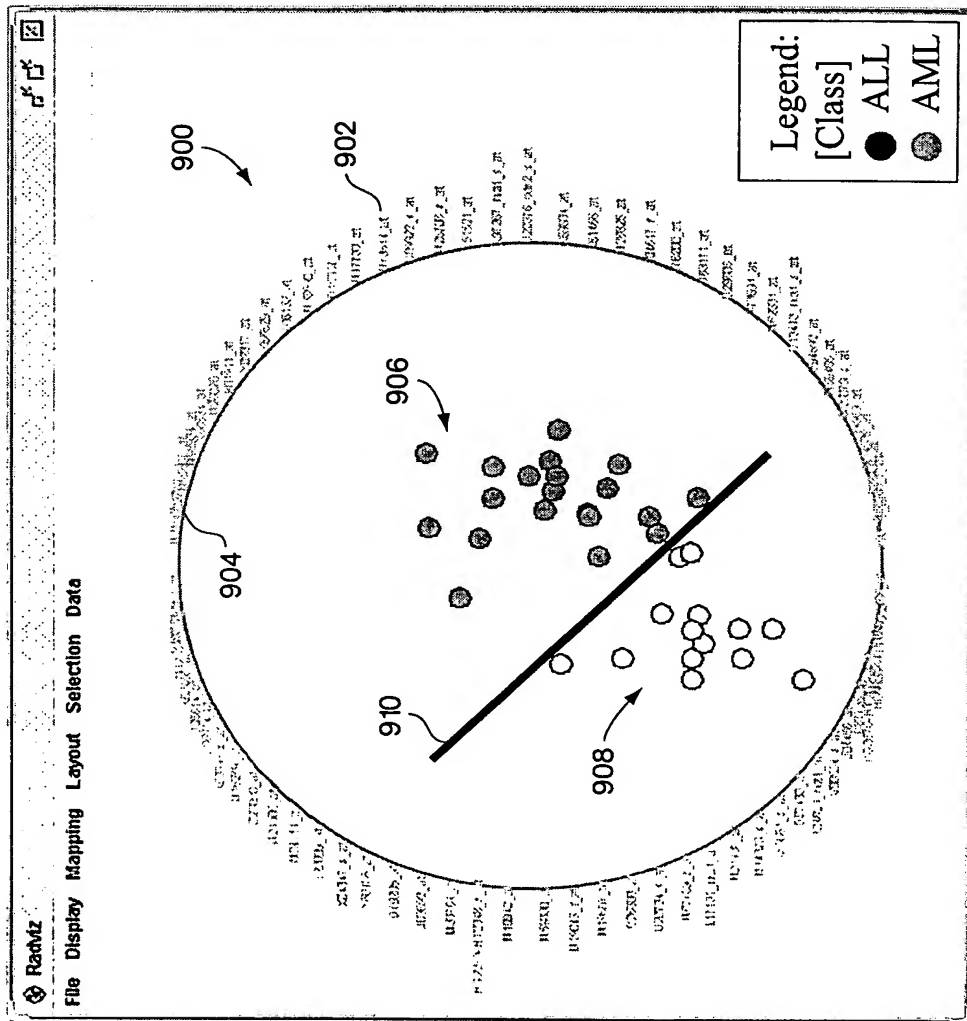Inventors: Grinstein, et al.
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Fig. 6E

Fig. 6F

Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
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Fig. 6G

Title: Method and System for Data Analy[...]
Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

Fig. 6H

: Method and System for Data Analys

Serial No.: 10/077,694
Inventors: Grinstein, et al.
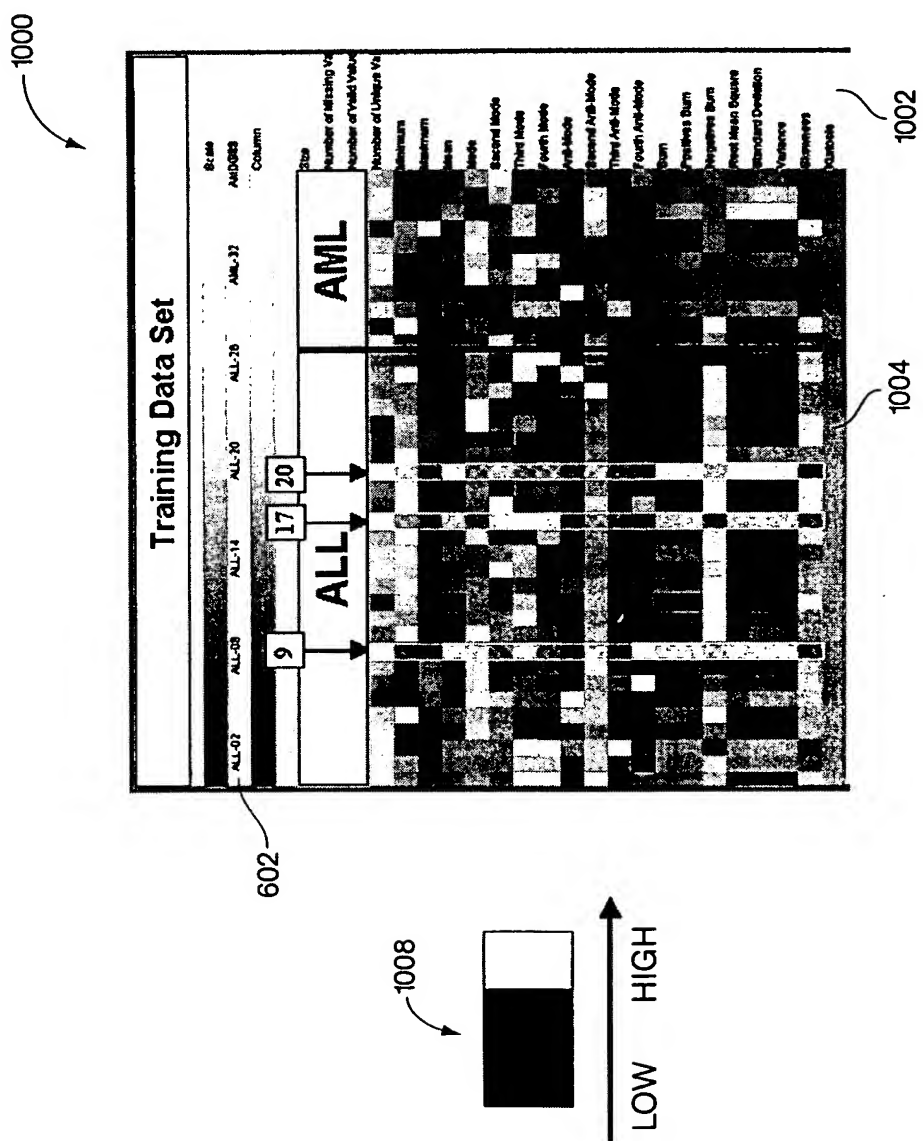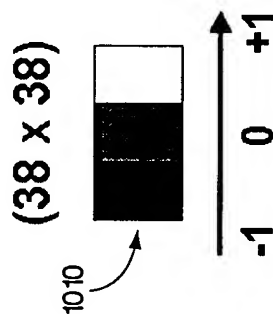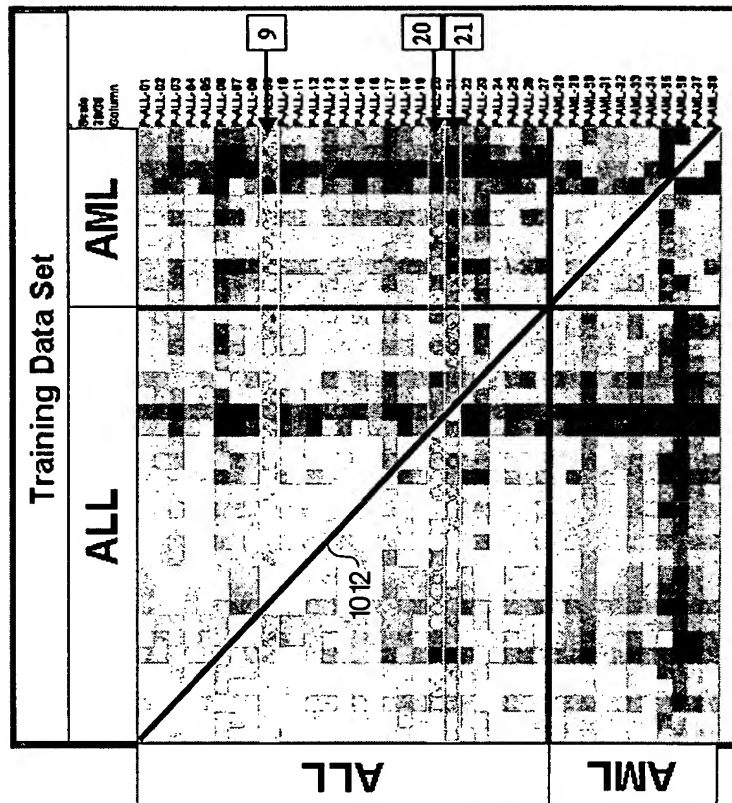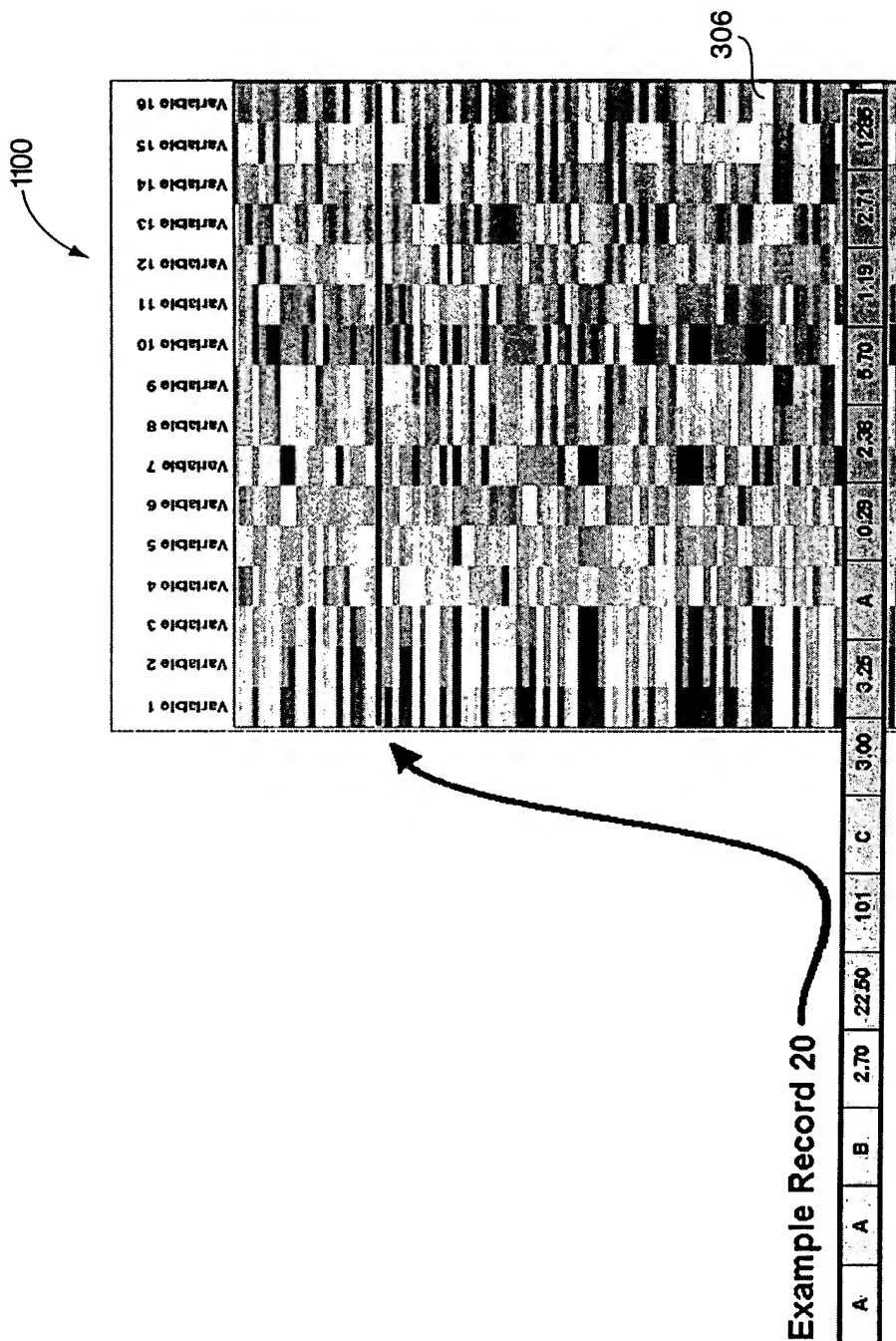Atty. Docket No.: ANVI-P01-001

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Fig. 7

Method and System for Data Analy...
...al No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

800

802 — ACCESS DATA

804 — ASSIGN 1D VECTORS

806 — SELECT OR RECEIVE K

808 — SELECT OR RECEIVE THRESHOLD

810 — SELECT OR RECEIVE INCREMENT

812 — CHOOSE FIRST VECTOR AT RANDOM

820 — SELECT ADDITIONAL VECTOR

822 — COMPUTE CORRELATION PARAMETER

824 — $T < CP$

NO

YES

826 — ADD ADDITIONAL VECTOR TO SUBSET

828 — DISCARD ADDITIONAL VECTOR

840 — HAVE ALL VECTORS BEEN TESTED ?

NO

YES

842 — OPTIONAL TEST: MORE THAN K VECTORS IN SUBSET ?

850 — ACCEPT SUBSET

NO

YES

844 — DECREMENT THRESHOLD BY THE INCREMENT VALUE AND REPEAT PROCESS FROM STEP 812 N TIMES
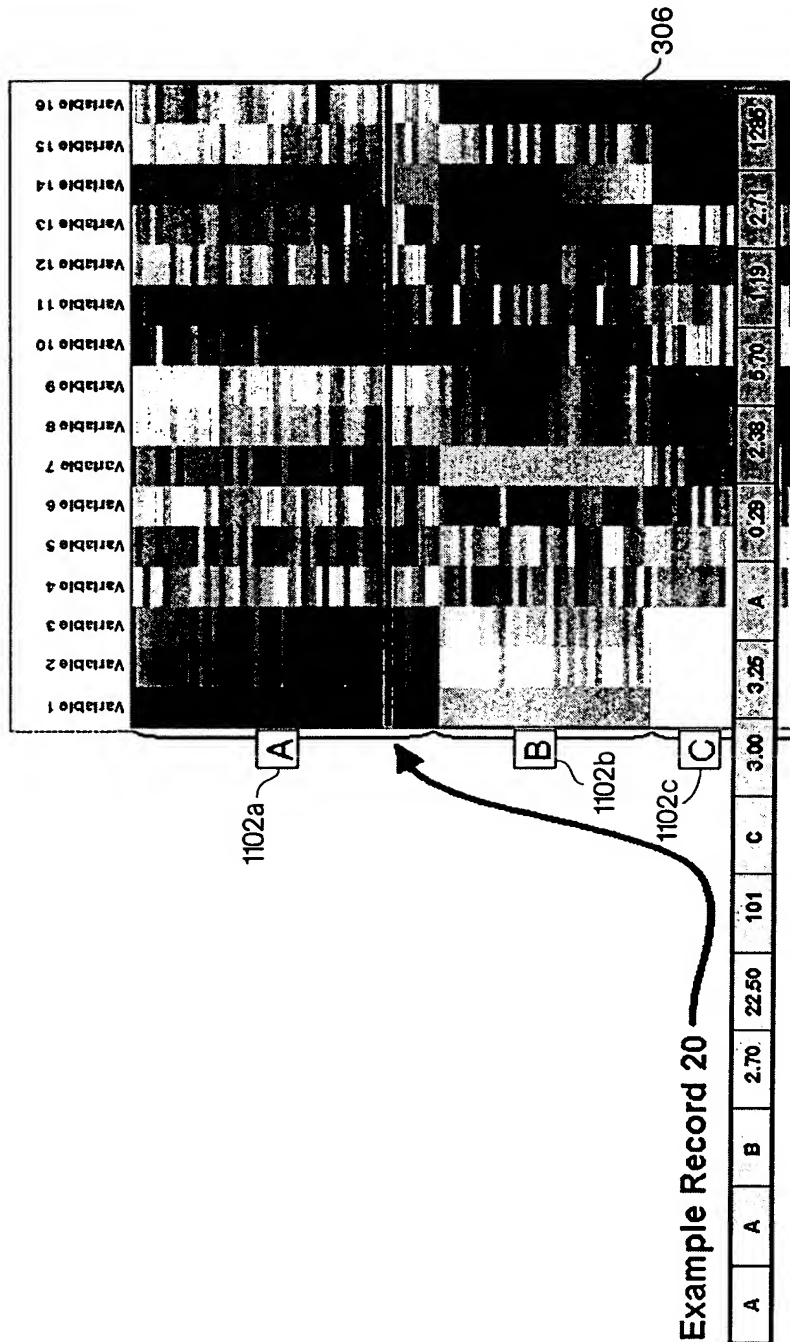
Fig. 8

RECEIVED
JUL 3 1 2002
Technology Center 2100

Method and System for Data Analysis
Serial No.: 10/077,694
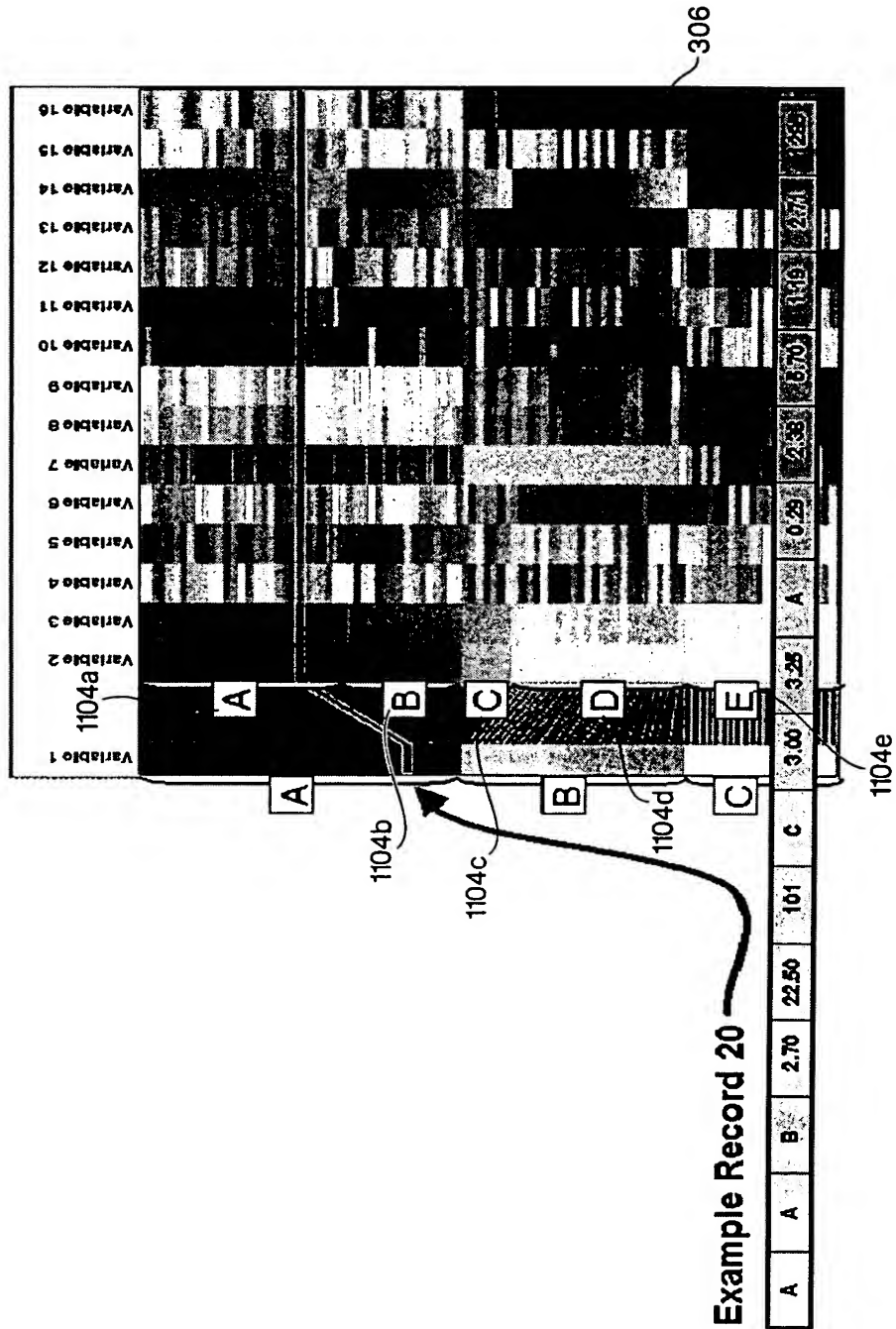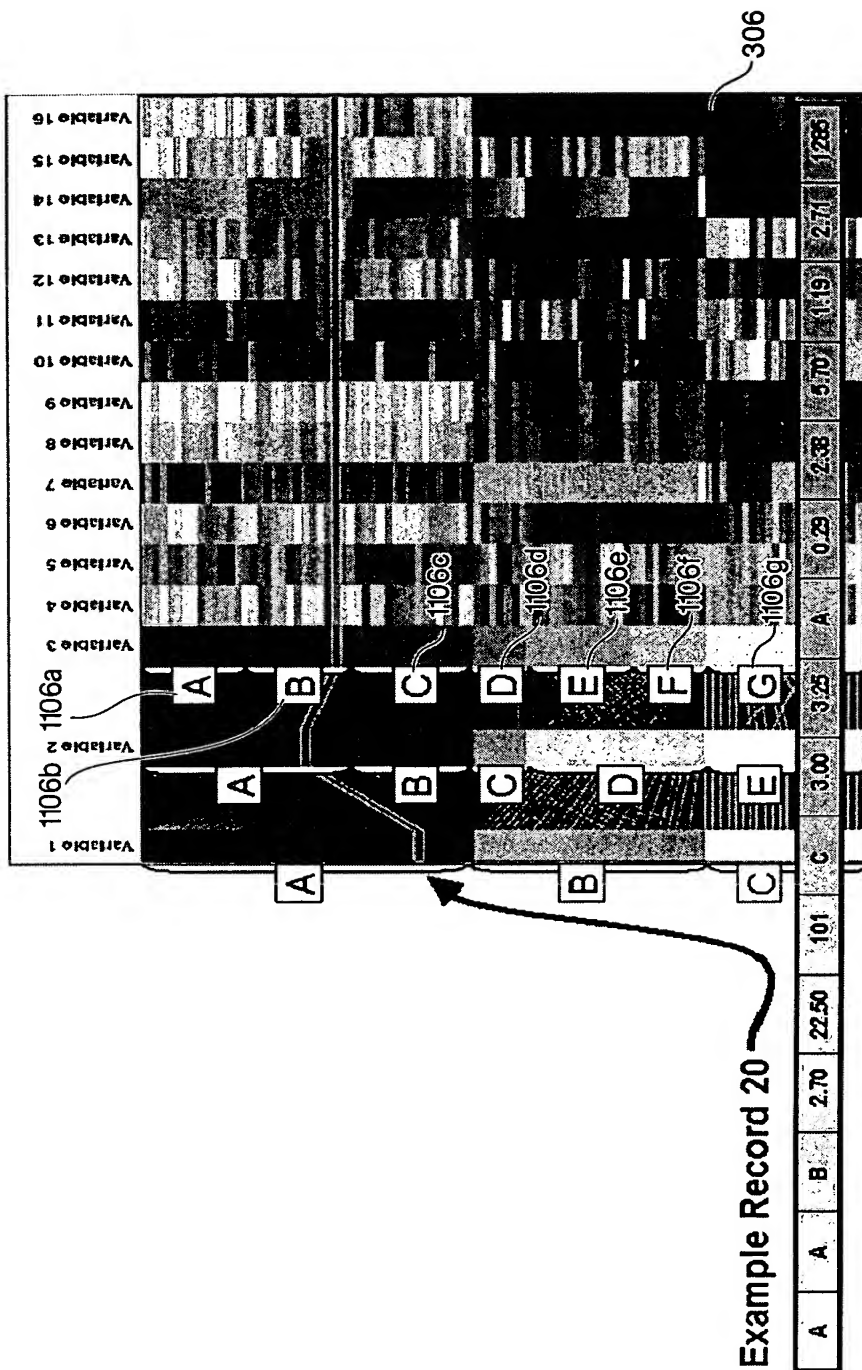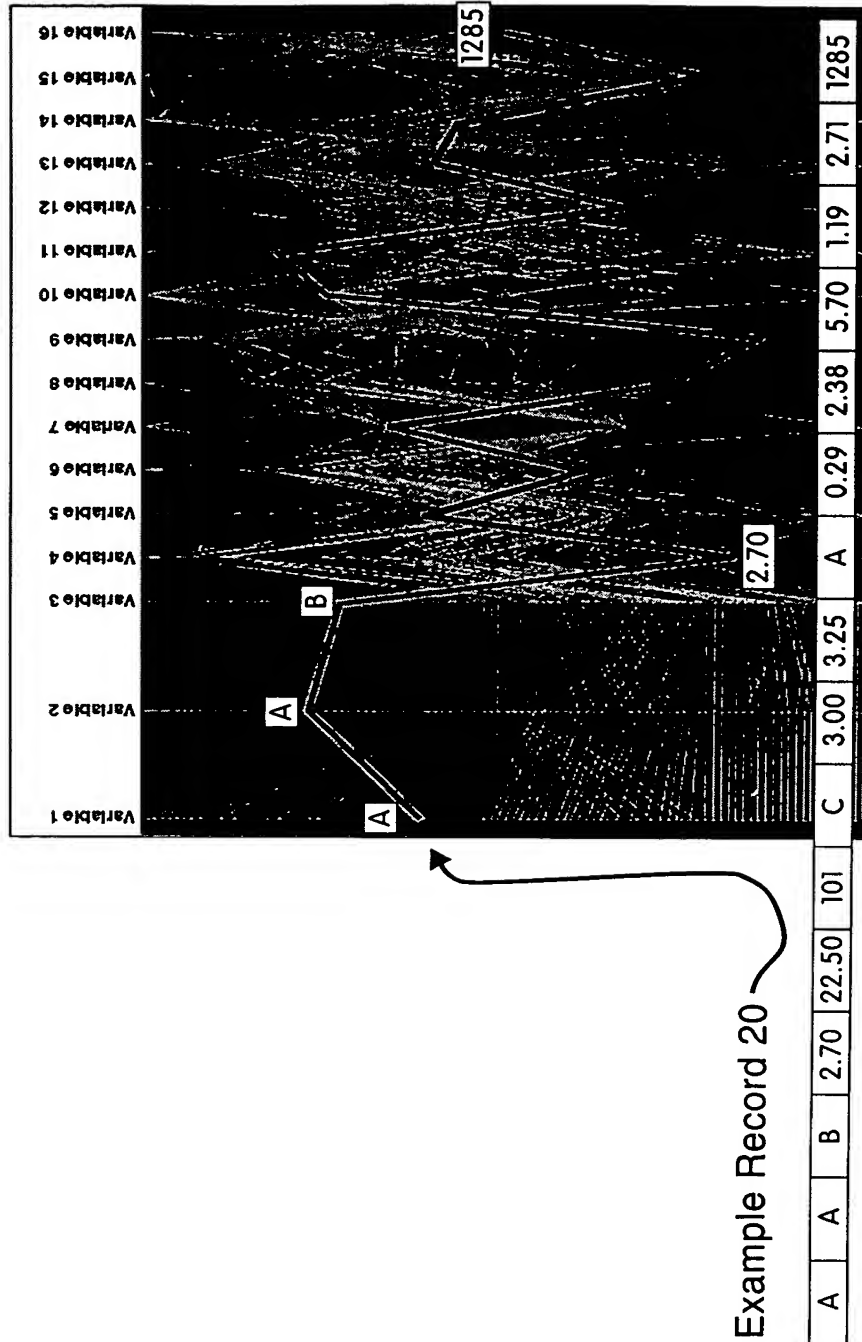Inventors: Grinstein, et al.
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Fig. 9

1000

1002

1004

602

1008

Training Data Set

AML

ALL

Fig. 10A

HIGH

LOW

Title: Method and System for Data Analysis
Serial No.: 10/077,694
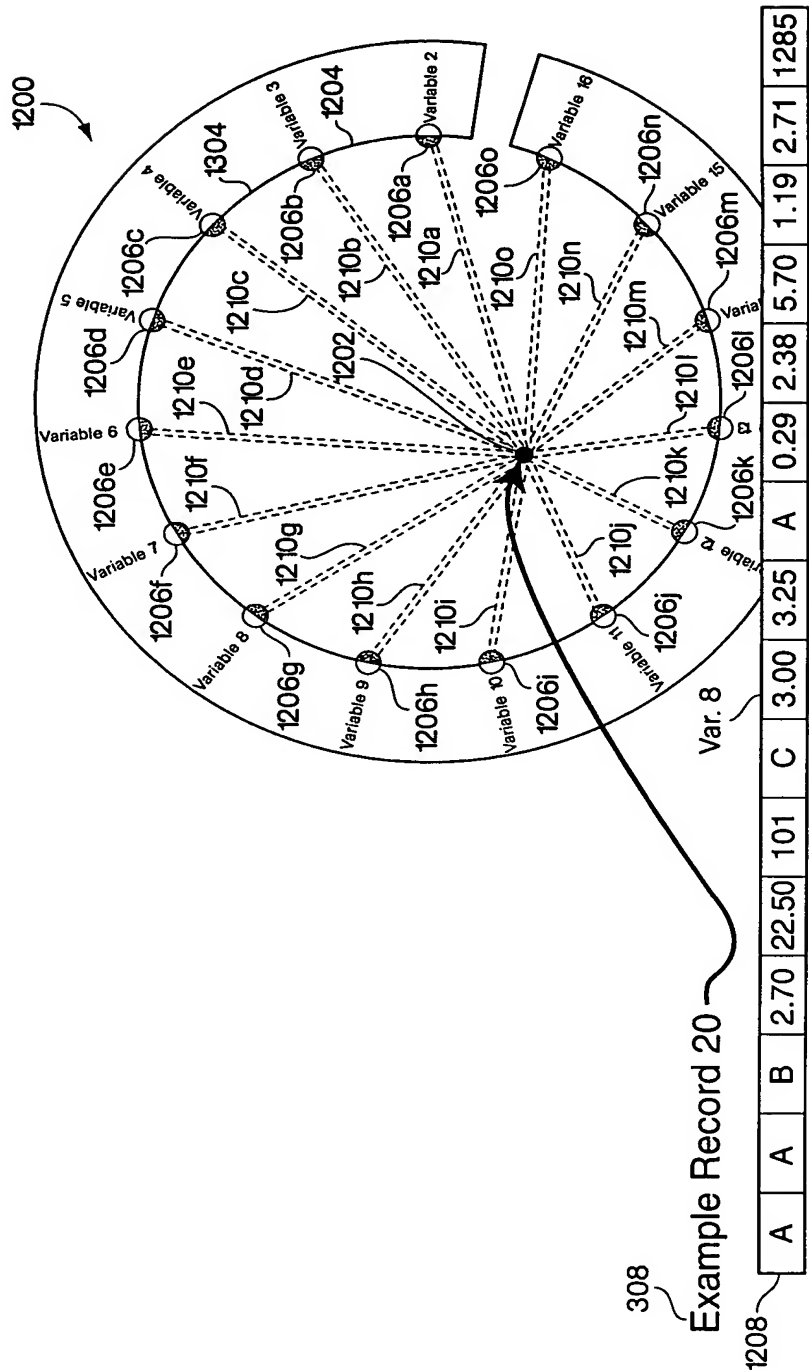Inventors: Grinstein, et al.
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Fig. 10B

Title Method and System for Data Analysis
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Fig. 10C

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Fig. 11A

Fig. 11B

Example Record 20

Title: Method and System for Data Analysis
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Fig. 11C

Example Record 20

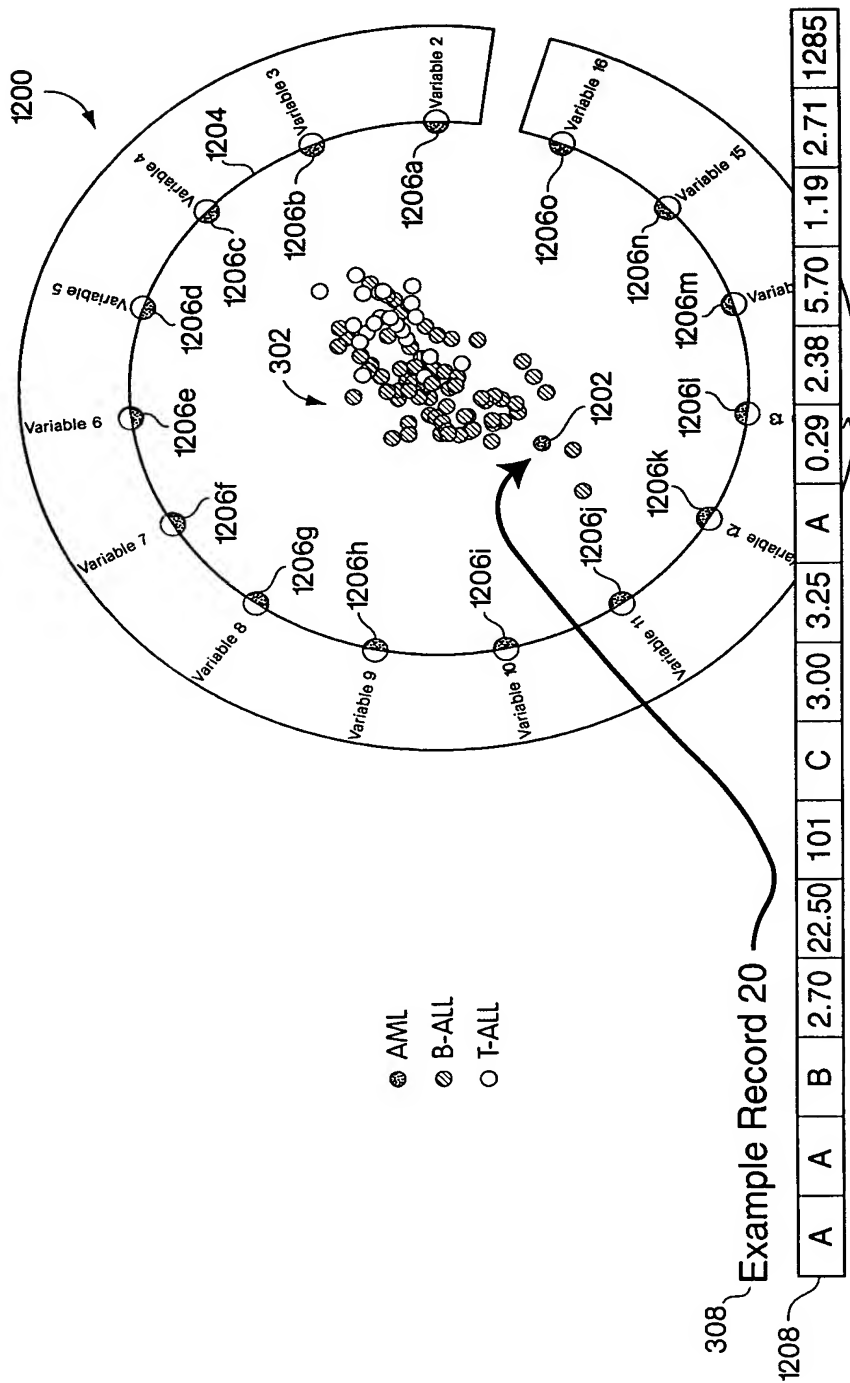Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

Fig. 11D

Title: Method and System for Data Analysis
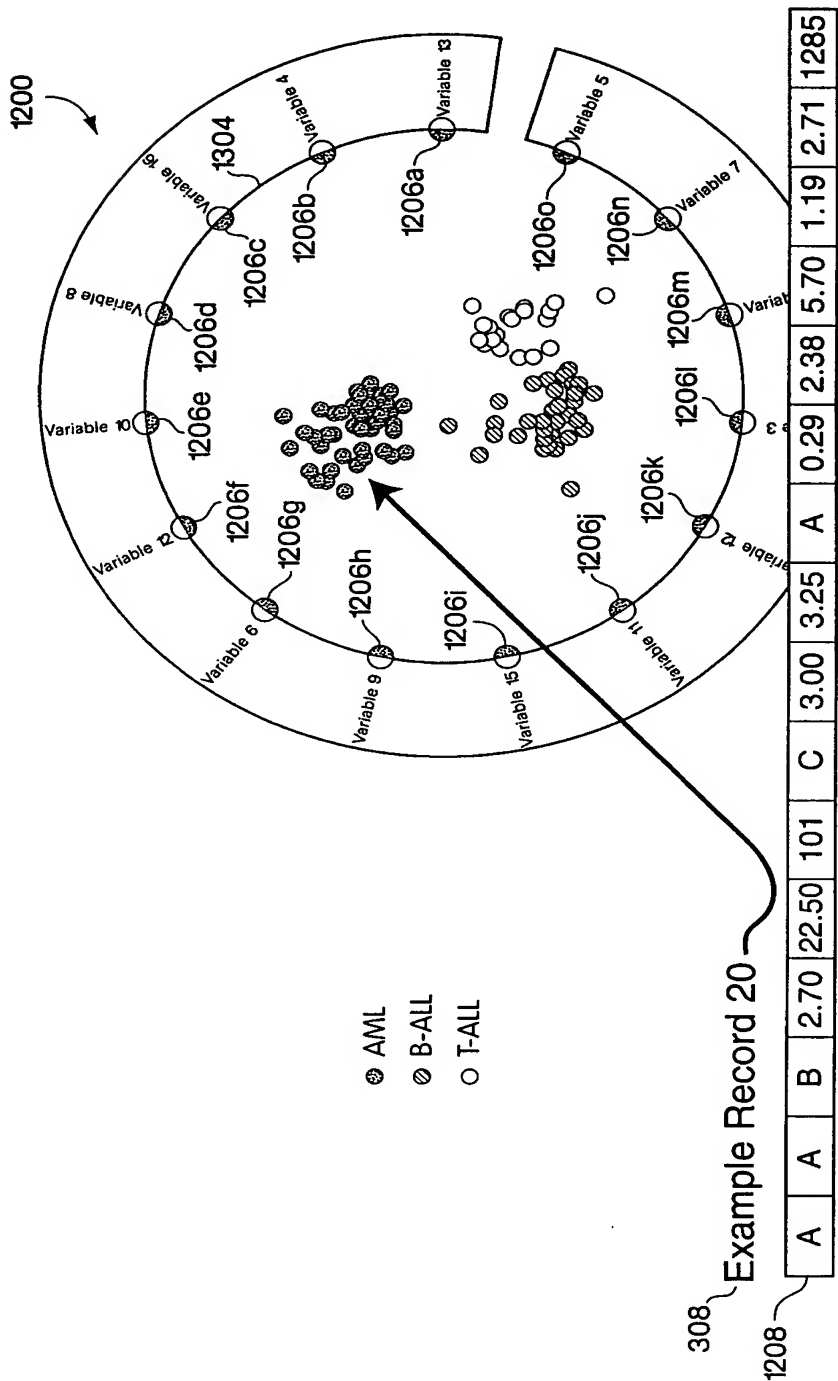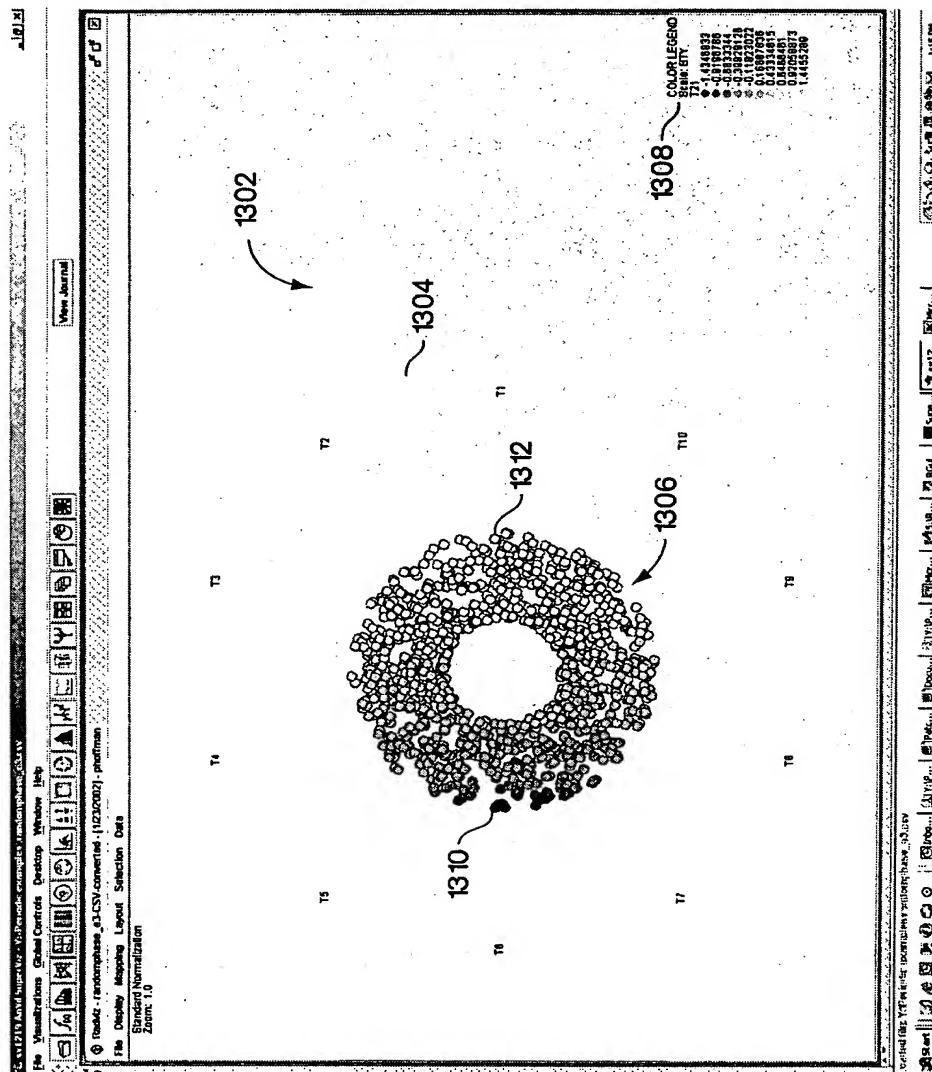Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 11E

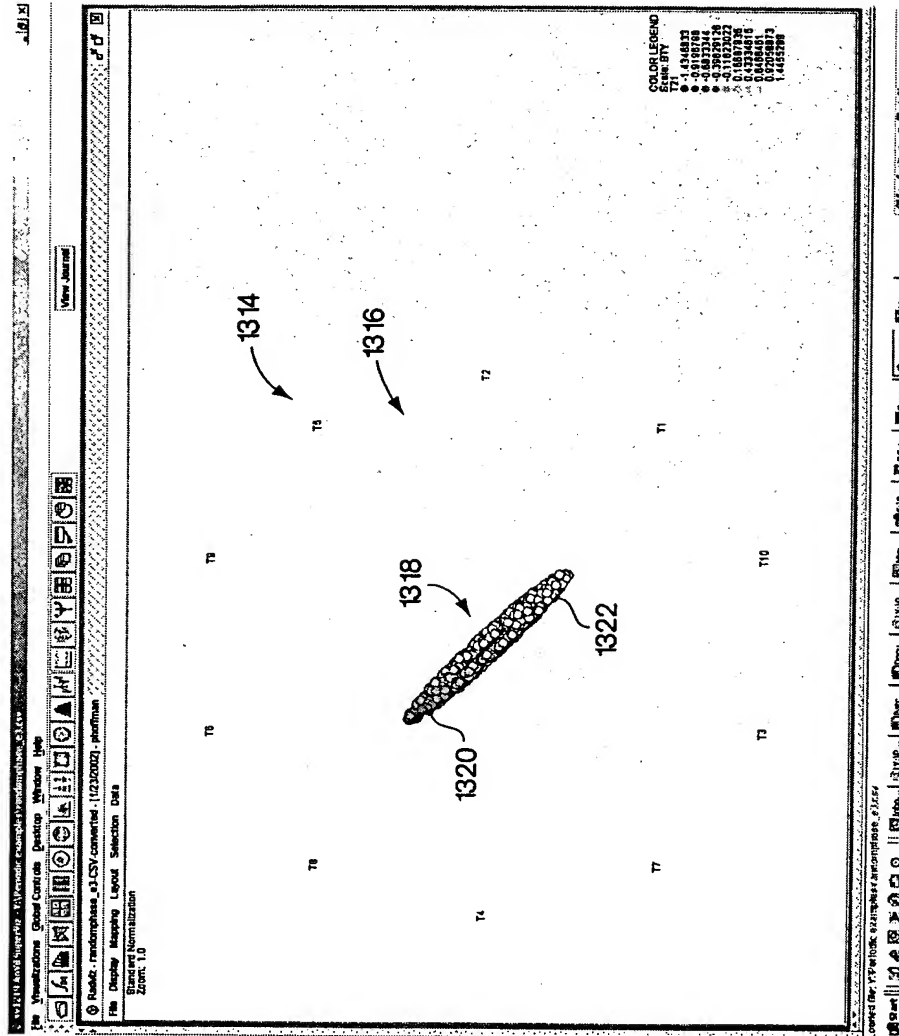Example Record 20

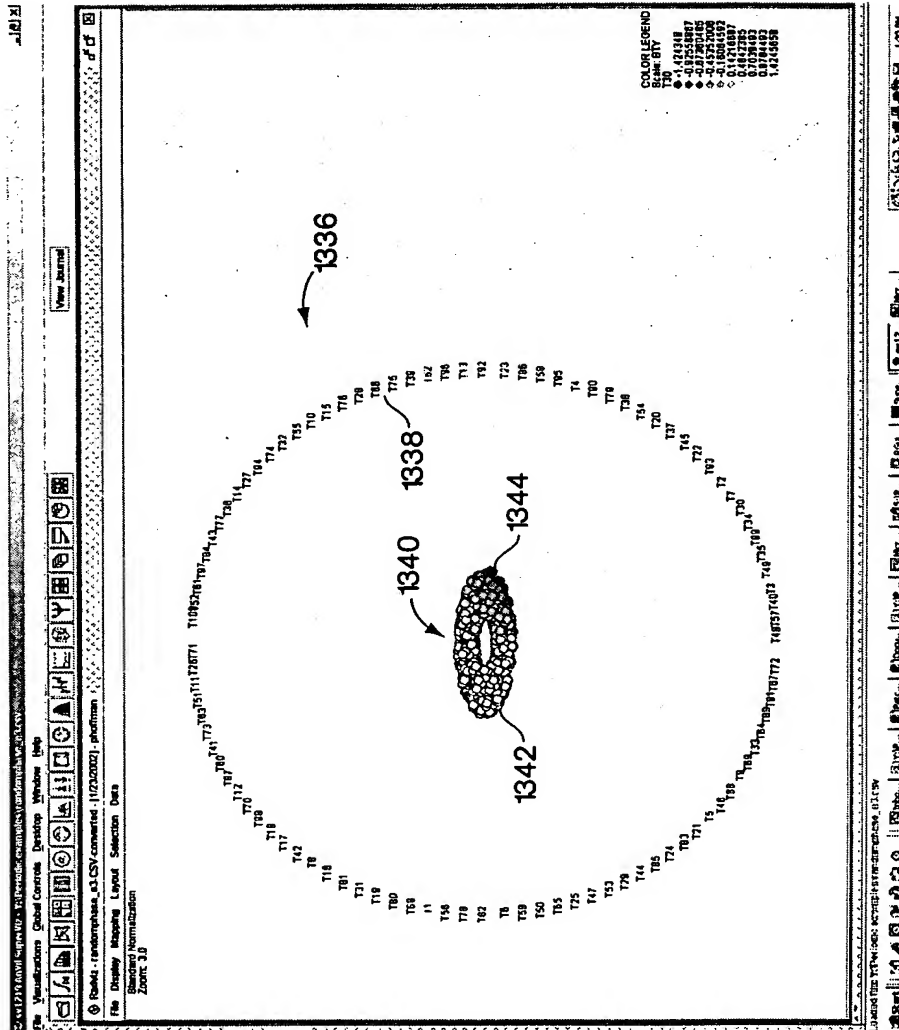| A | A | B | 2.70 | 22.50 | 101 | C | 3.00 | 3.25 | A | 2.70 | 0.29 | 2.38 | 5.70 | 1.19 | 2.71 | 1285 |

Method and System for Data Analysis
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Fig. 12A

The Method and System for Data Analysis
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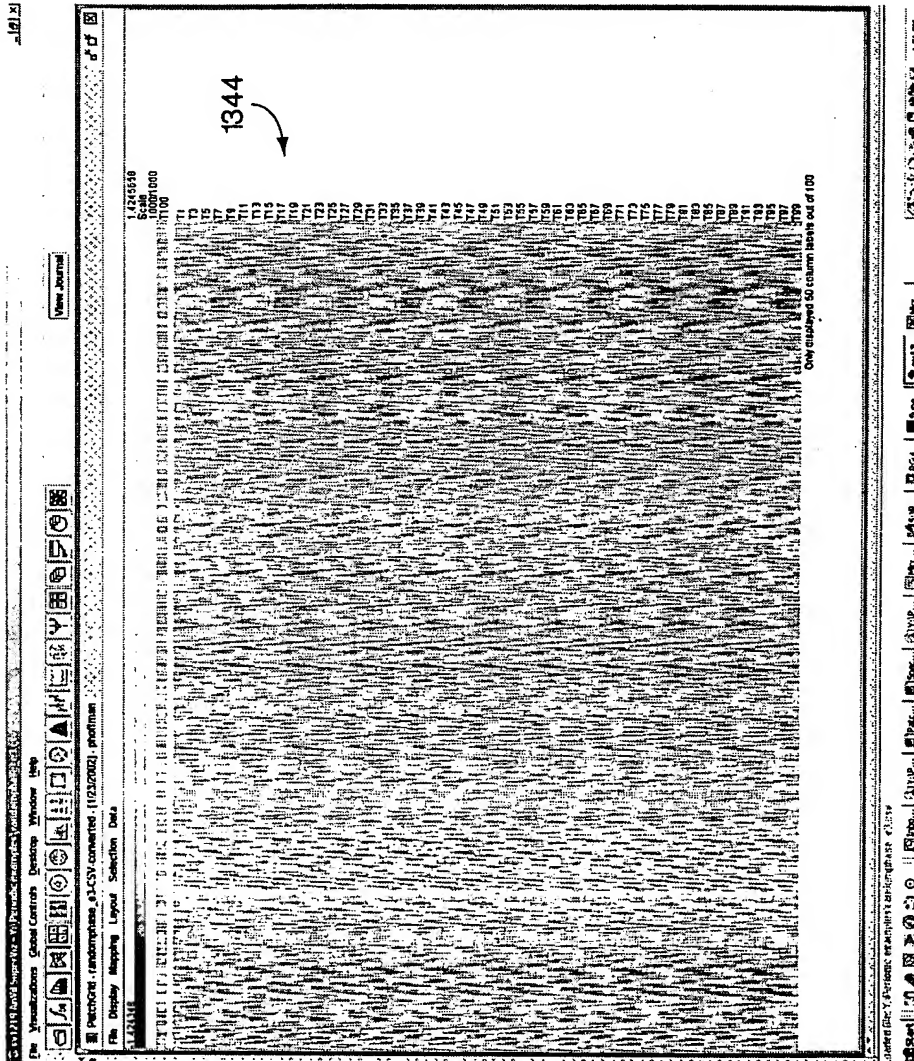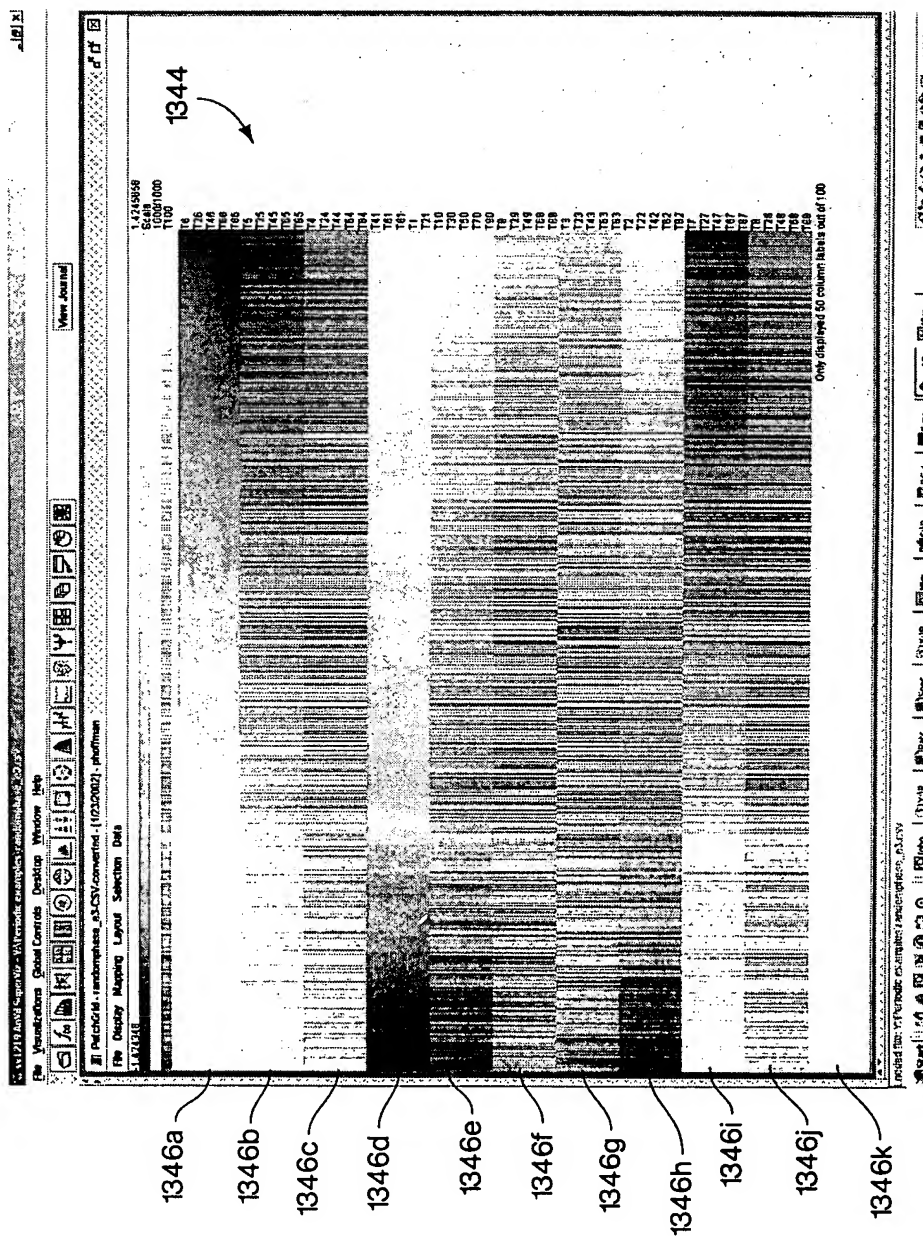Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 12B

A	A	B	A	A	C	3.00	3.25	A	0.29	2.38	5.70	1.19	2.71	1285
		2.70	22.50	101										

Example Record 20

⊕ AML
⊘ B-ALL
○ T-ALL

Fig. 12C

308	Example Record 20

1208	A	A	B	C	C	A	A	0.29	2.38	5.70	1.19	2.71	1285

Legend:
- ⊕ AML
- ⊘ B-ALL
- ○ T-ALL

Method and System for Data Analysis
Serial No.: 10/077,694
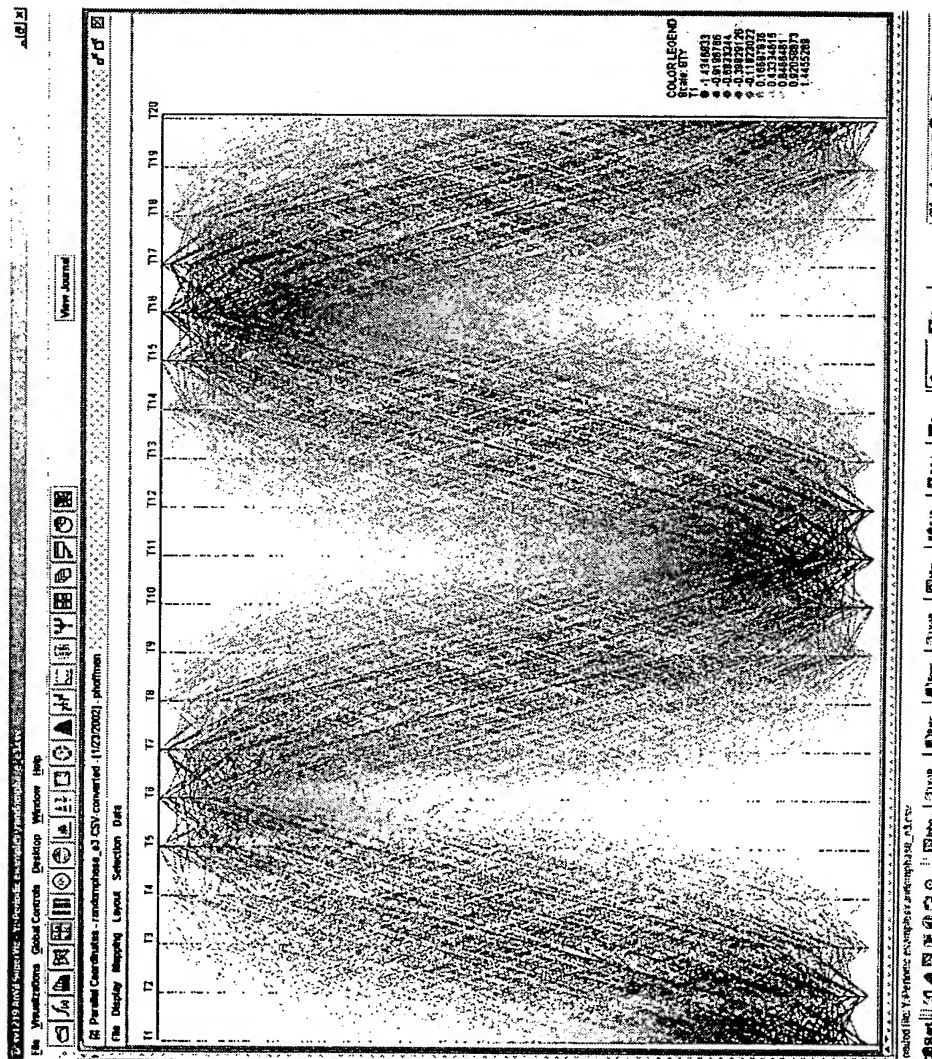Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

Fig. 13A

Title: Method and System for Data Analysis
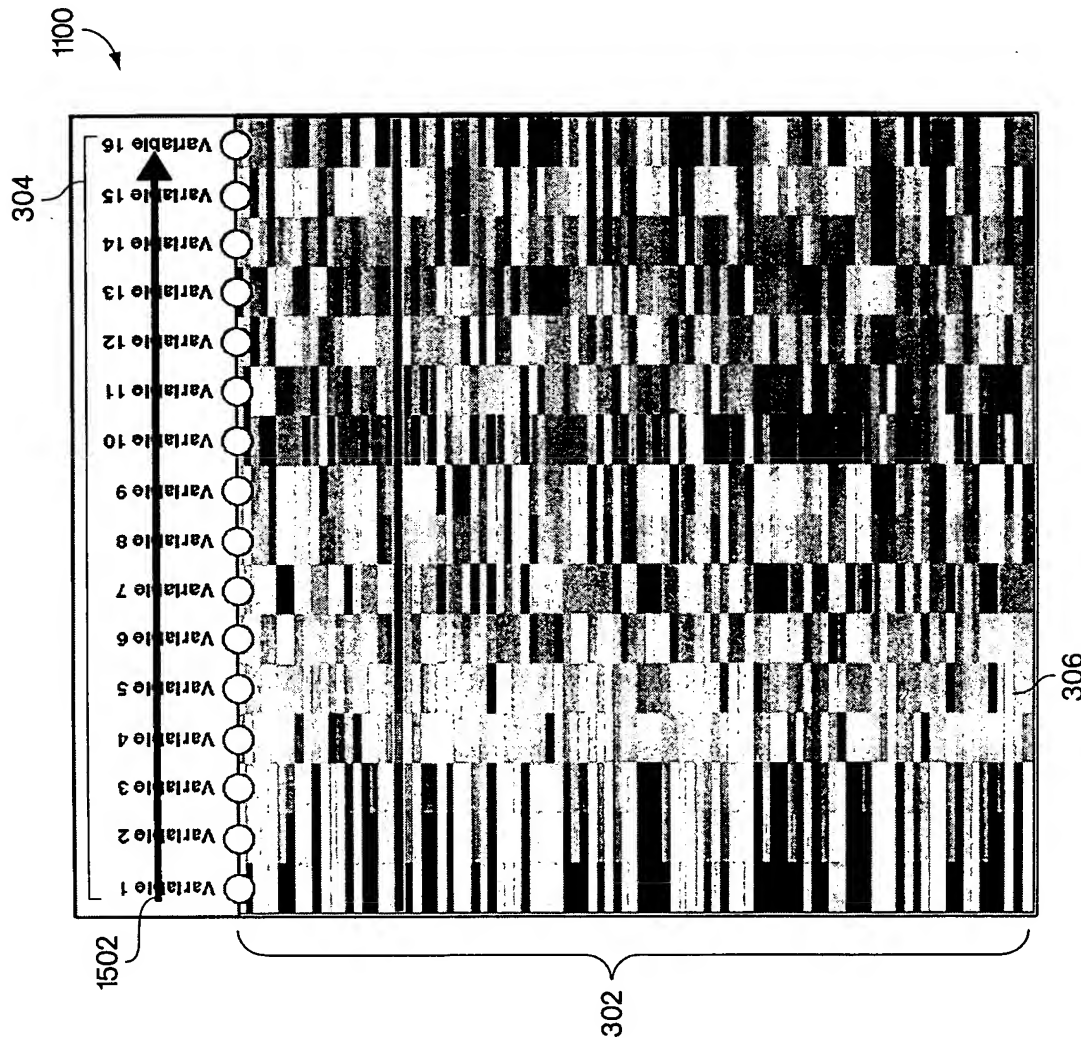Serial No.: 10/077,694
Inventors: Grinstein, et al.
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Fig. 13B

Fig. 18C

: Method and System for Data Analysis
Serial No.: 10/077,694
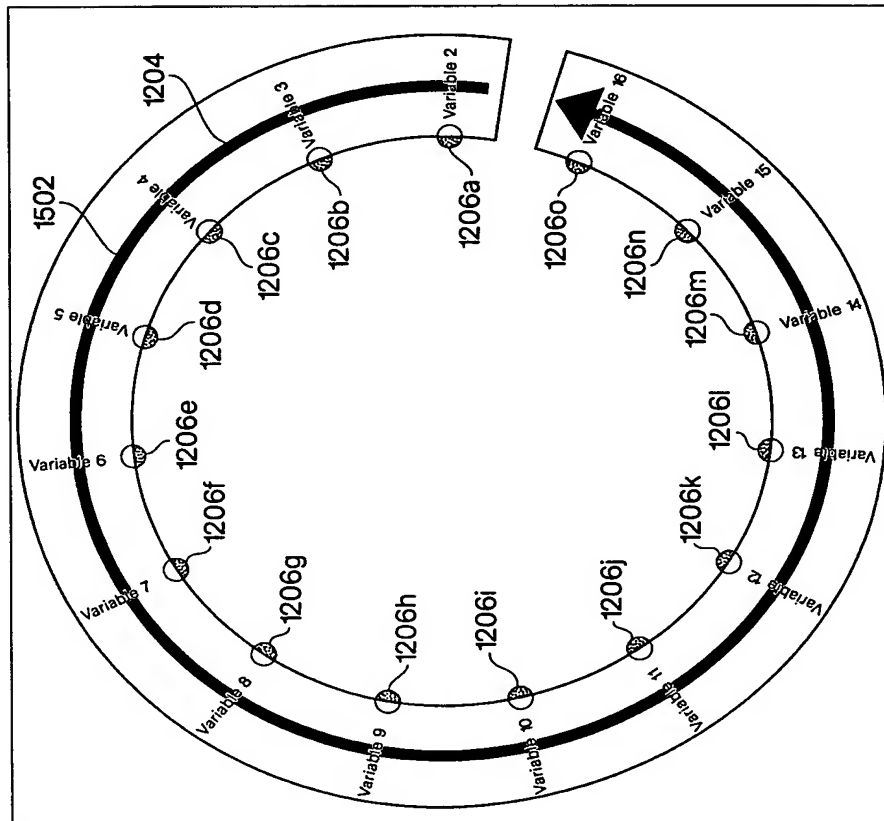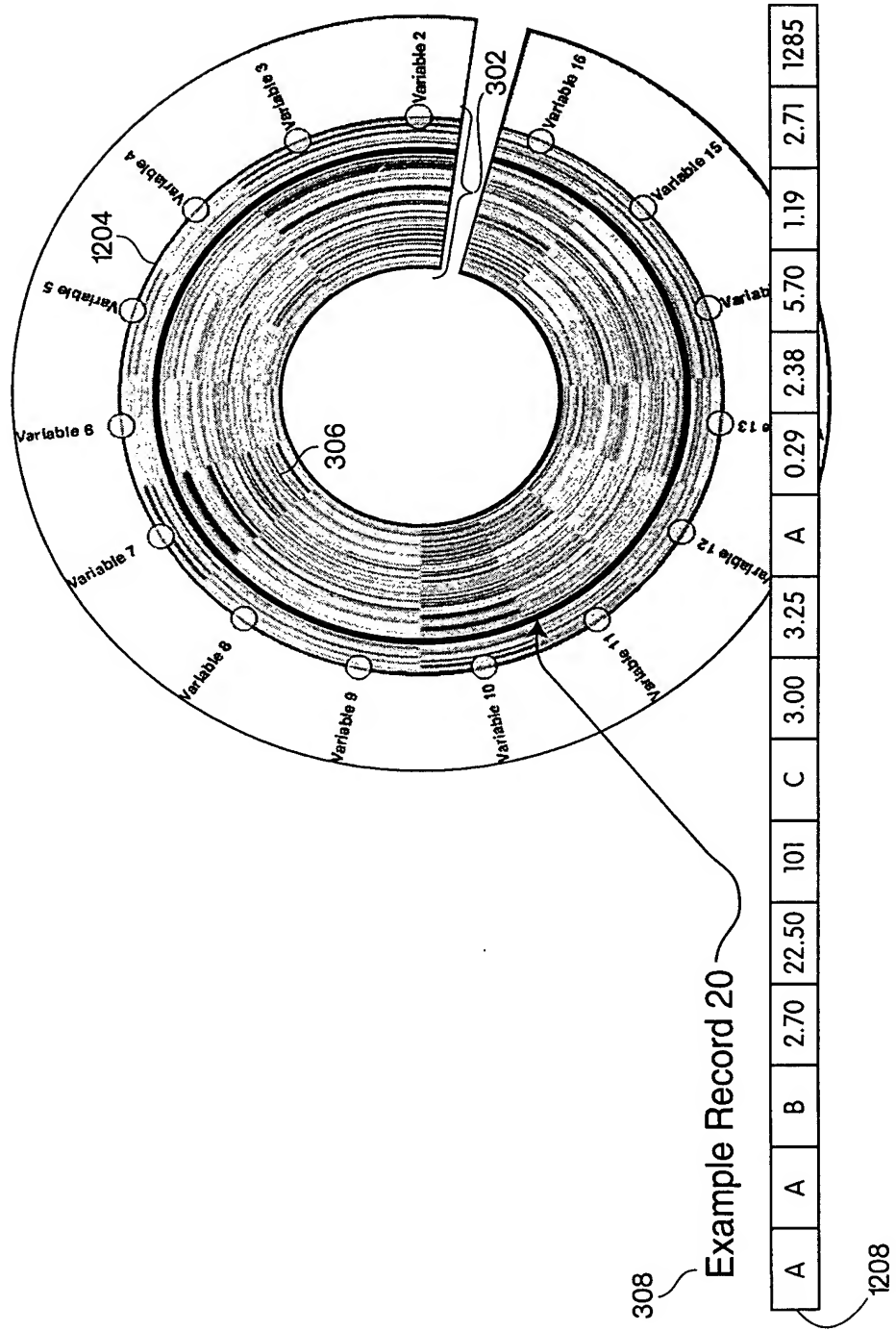Inventors: Grinstein, et al.
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Fig. 13D

: Method and System for Data Analysis
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Inventors: Grinstein, et al.
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Fig. 14A

Title: Method and System for Data Analysis
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Inventors: Grinstein, et al.
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Fig. 14B

Title: Method and System for Data Analysis
Serial No.: 10/077,694
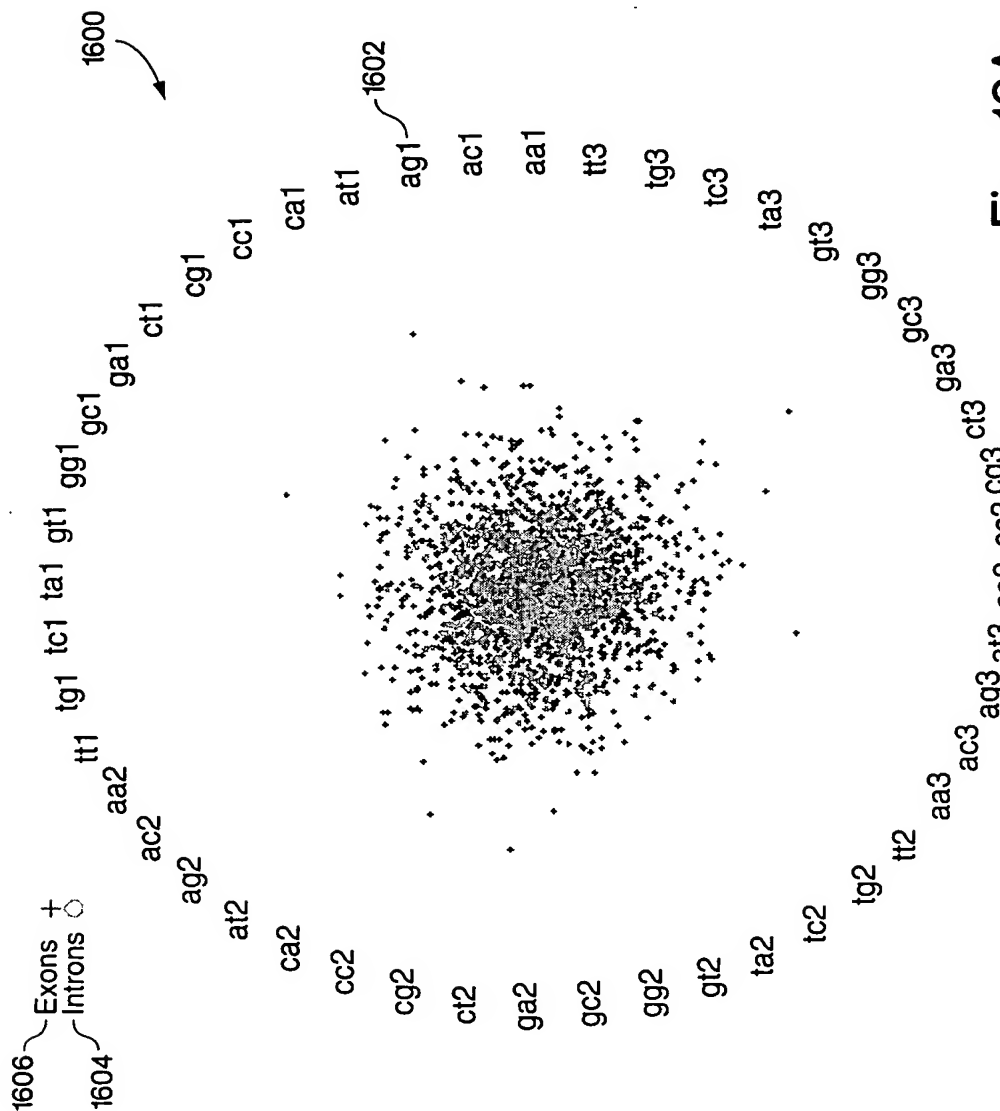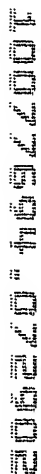Inventors: Grinstein, et al.
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Fig. 14C

Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
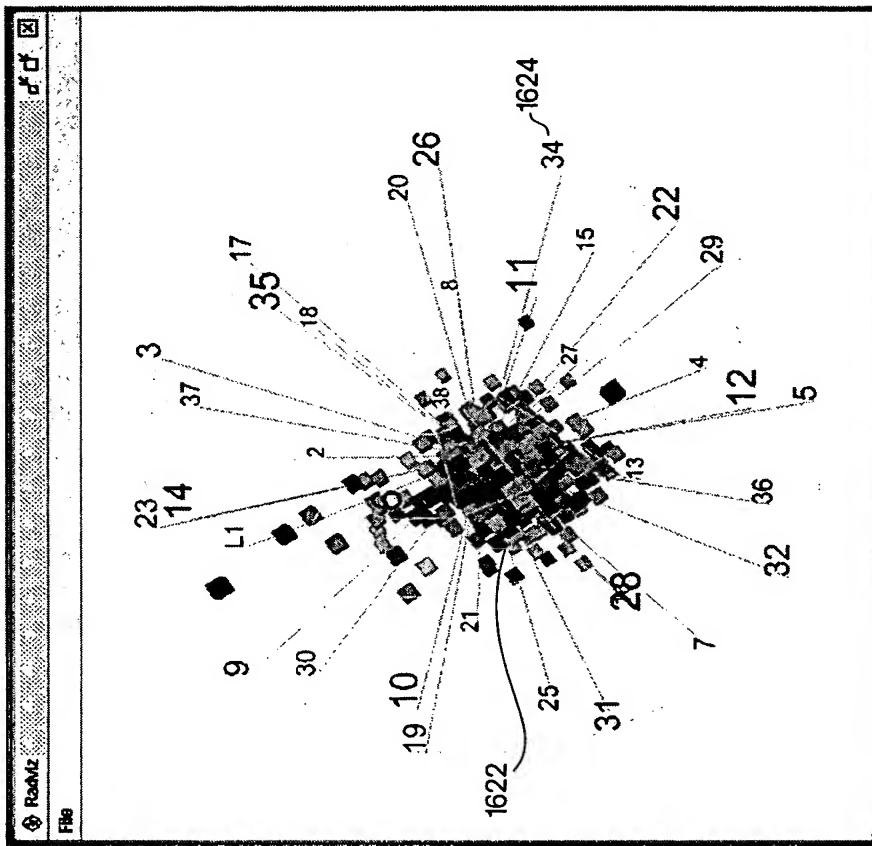Atty. Docket No.: ANVI-P01-001

Fig. 15A

Fig. 15B

Fig. 15C

A	A	B	2.70	22.50	101	C	3.00	3.25	A	0.29	2.38	5.70	1.19	2.71	1285

Example Record 20
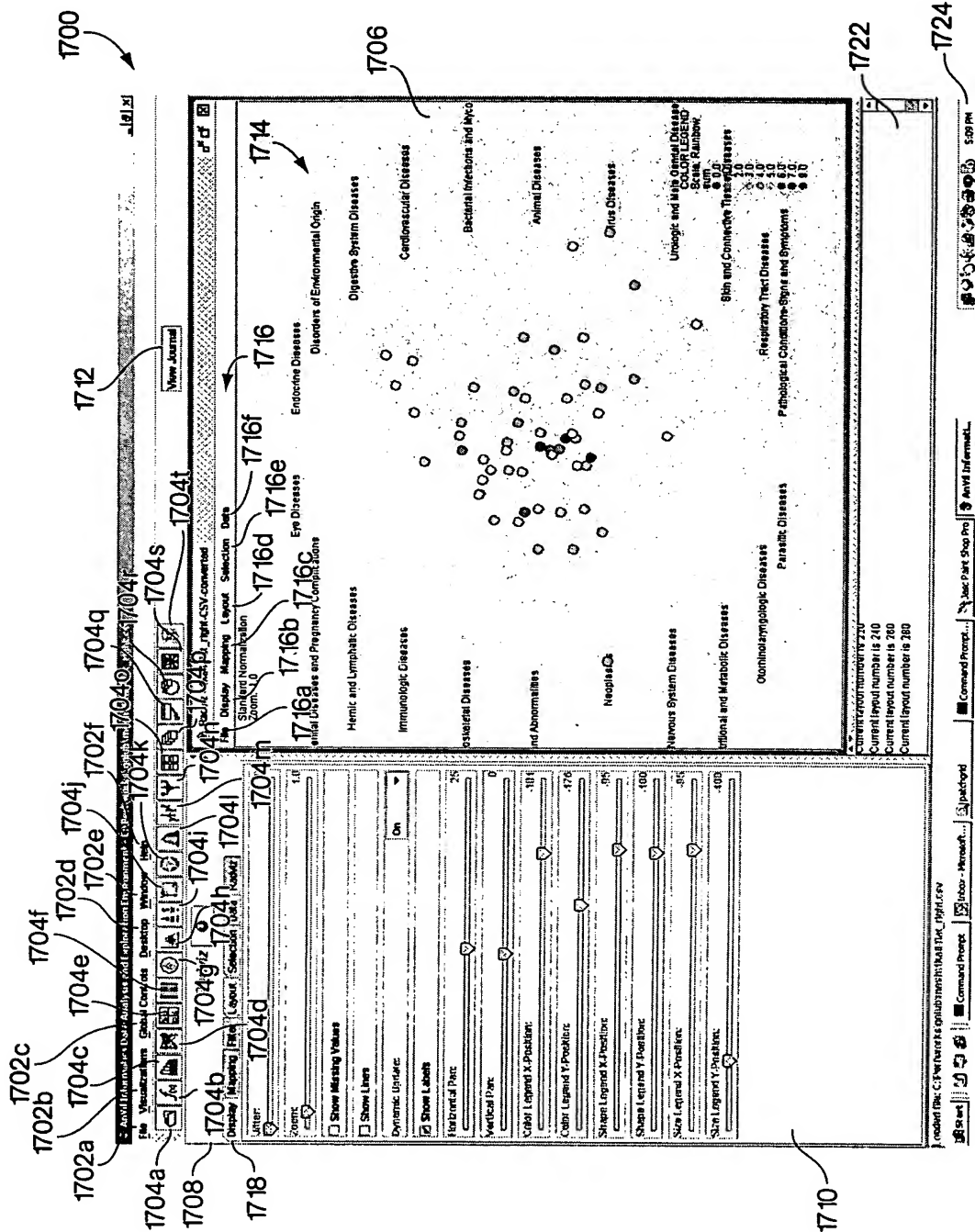
Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
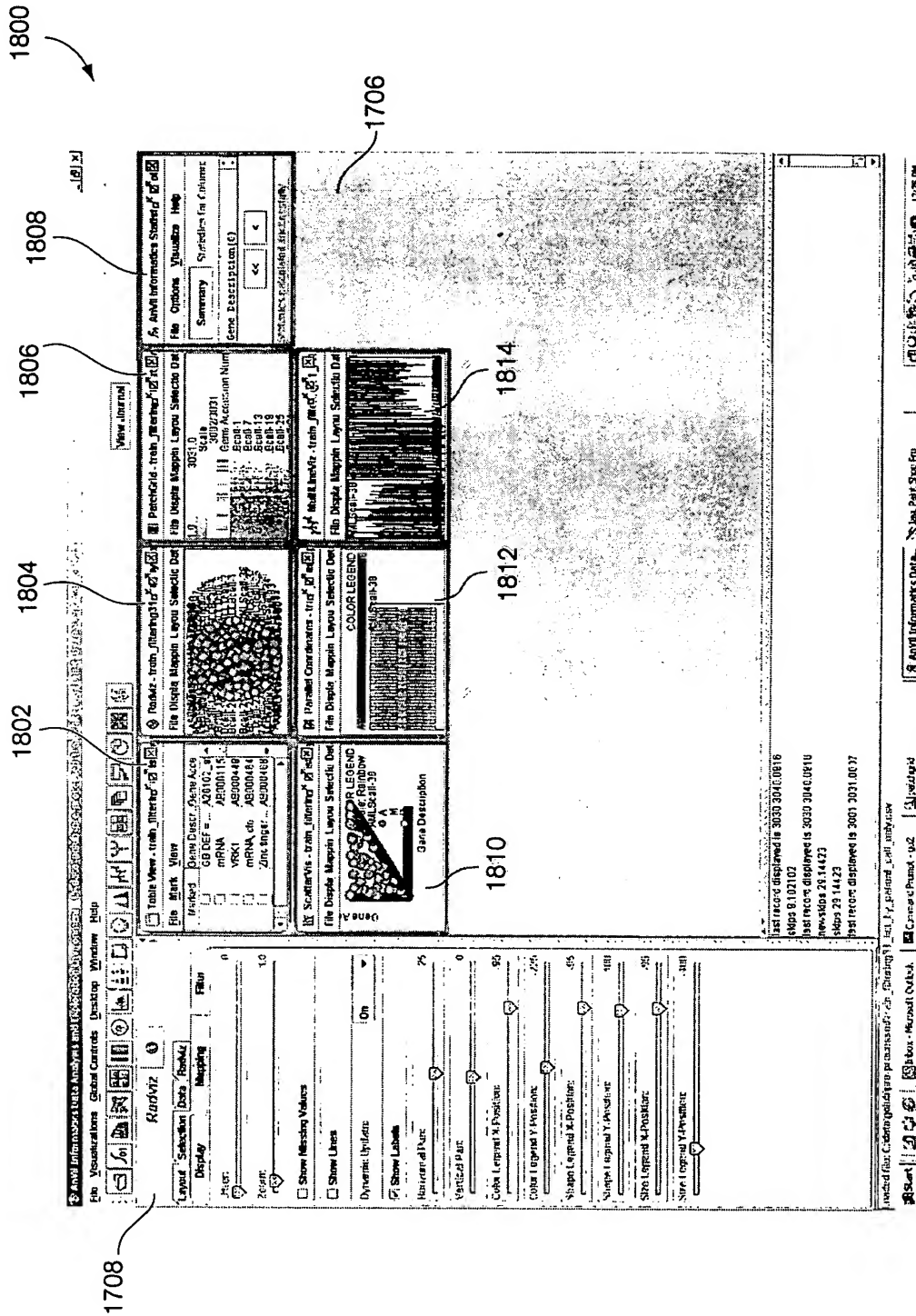Atty. Docket No.: ANVI-P01-001

Fig. 16A

Title: Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
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Fig. 16B

The Method and System for Data Analysis
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Fig. 16C

Title: Method and System for Data Analysis
Serial No.: 10/077,694
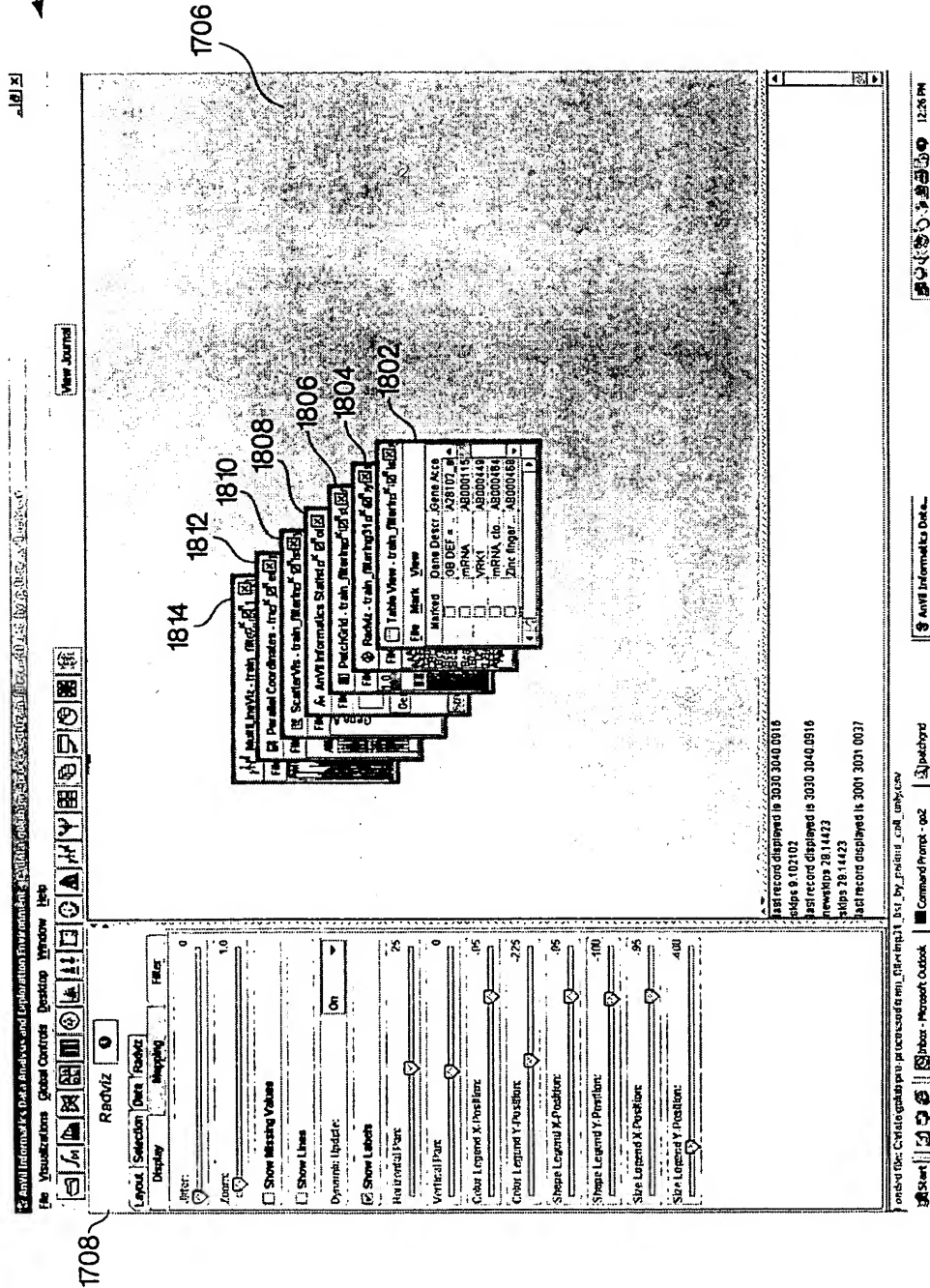Inventors: Grinstein, et al.
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Fig. 16D

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Inventors: Grinstein, et al.
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Fig. 17

Fig. 18

Method and System for Data Analysis
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Fig. 19

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Fig. 21

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Fig. 22

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e: Method and System for Data Analy
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Fig. 24

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Fig. 25

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Fig. 26

Title: Method and System for Data Analysis
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Fig. 27

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Fig. 28

The Method and System for Data Analysis
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Fig. 29

The Method and System for Data Analysis
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Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 30

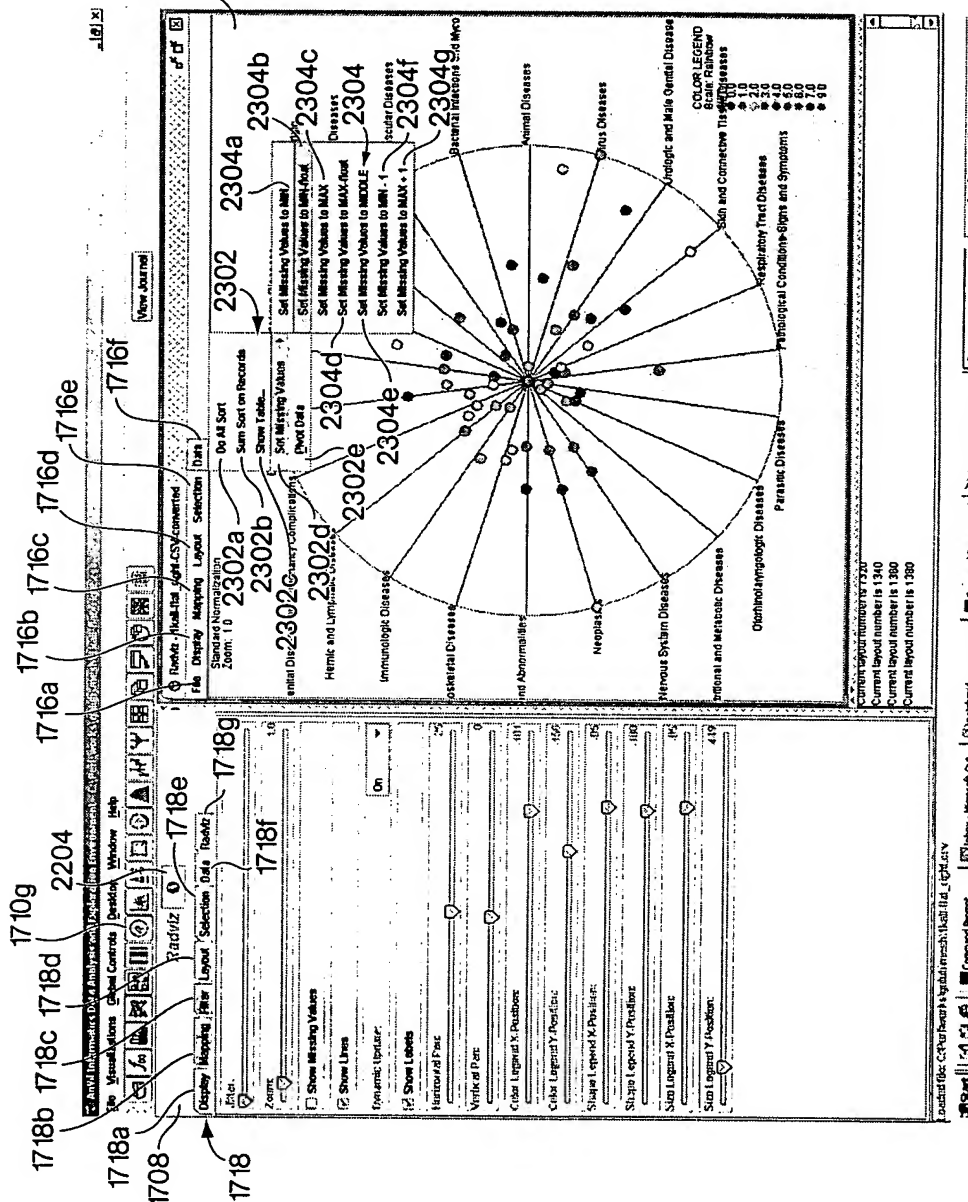Title: Method and System for Data Analysis
Serial No.: 10/077,694
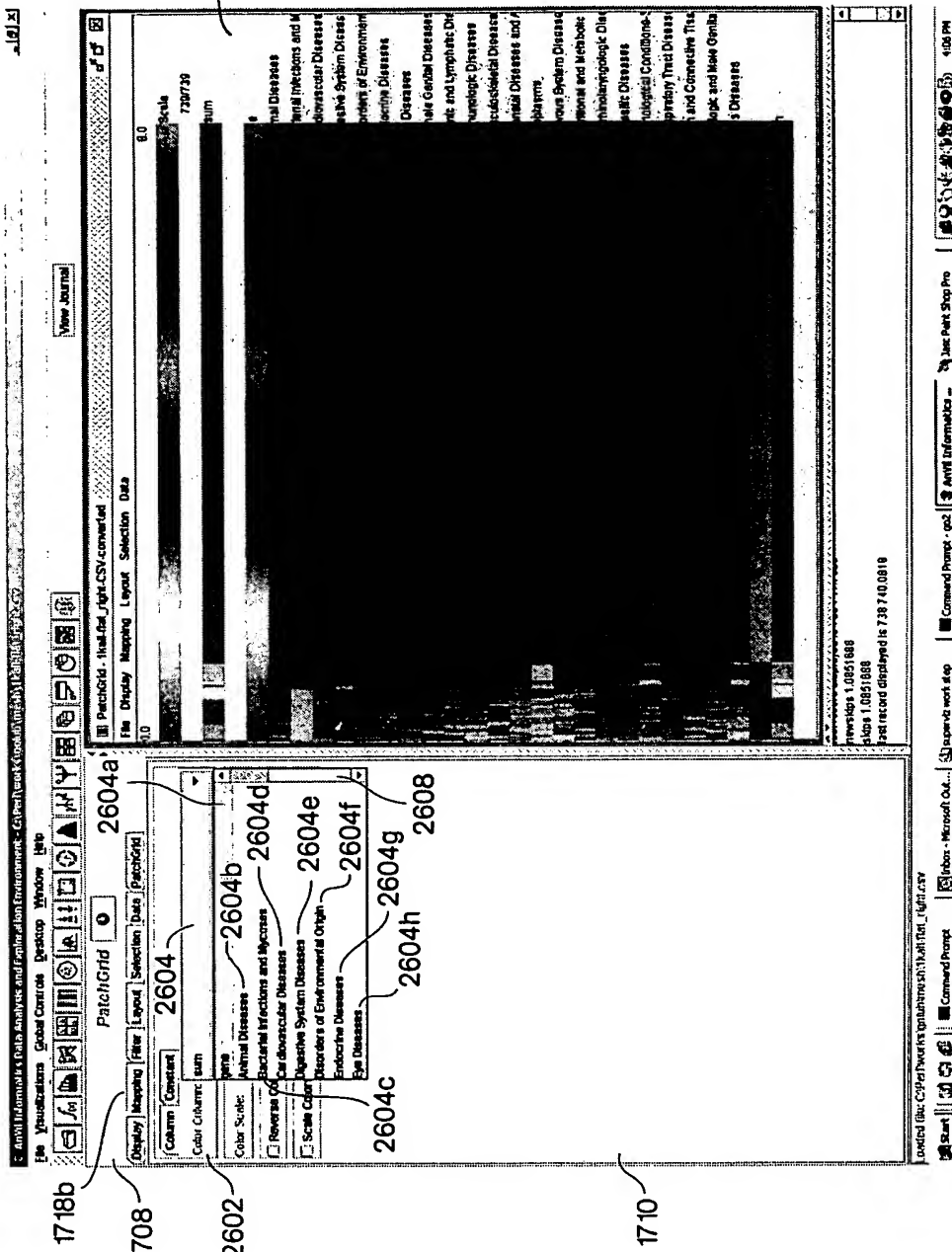Inventors: Grinstein, et al.
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Fig. 31

Title: Method and System for Data Analysis
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Inventors: Grinstein, et al.
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Fig. 32

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Fig. 33

Fig. 34

Fig. 35

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Fig. 36

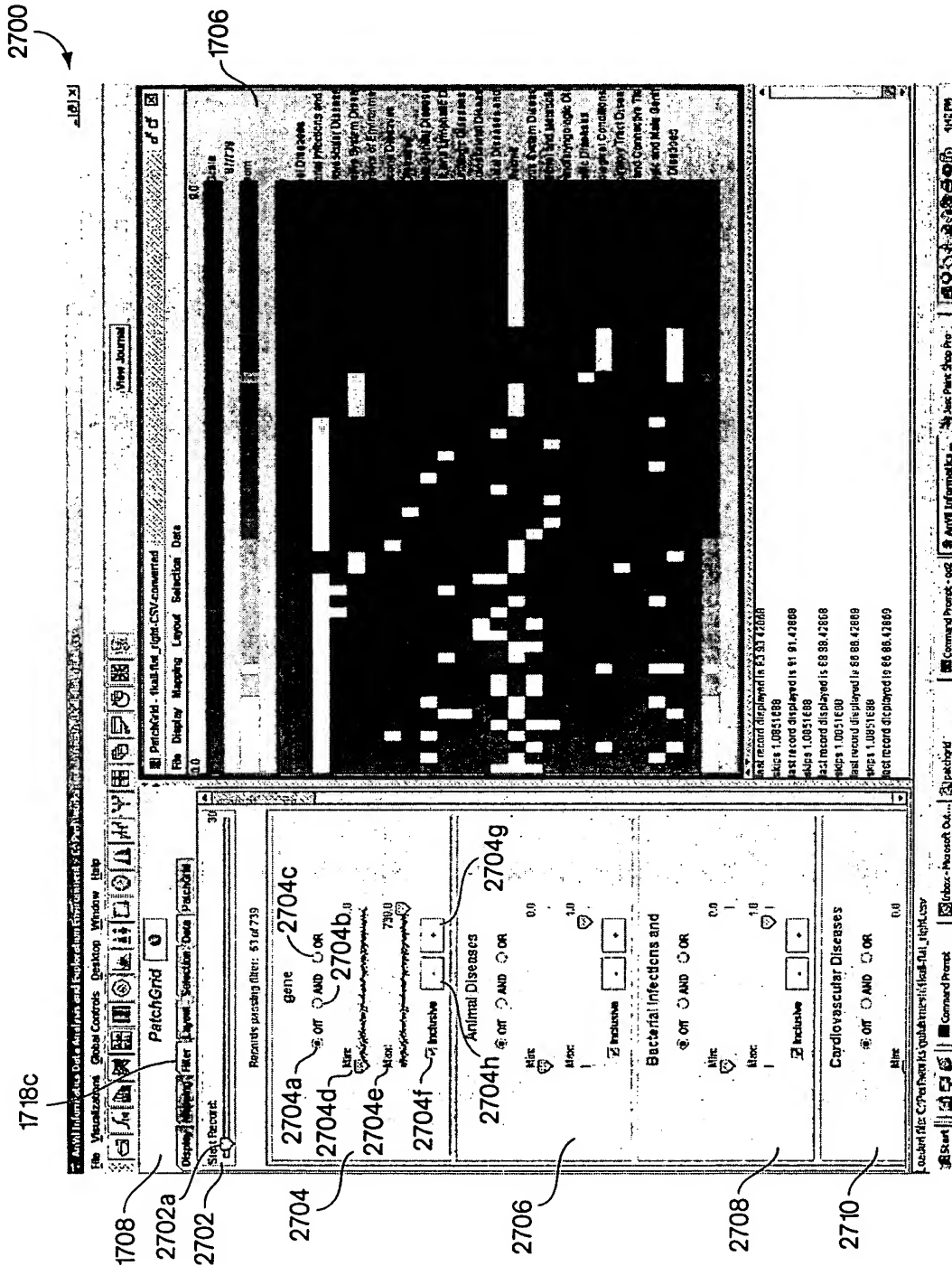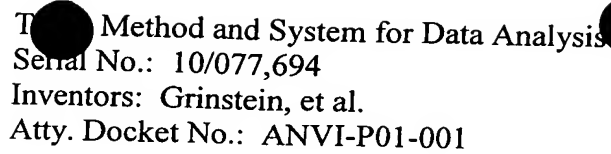Title: Method and System for Data Analy
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Fig. 37

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Fig. 38

Title: Method and System for Data Analysis
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Fig. 39

3800
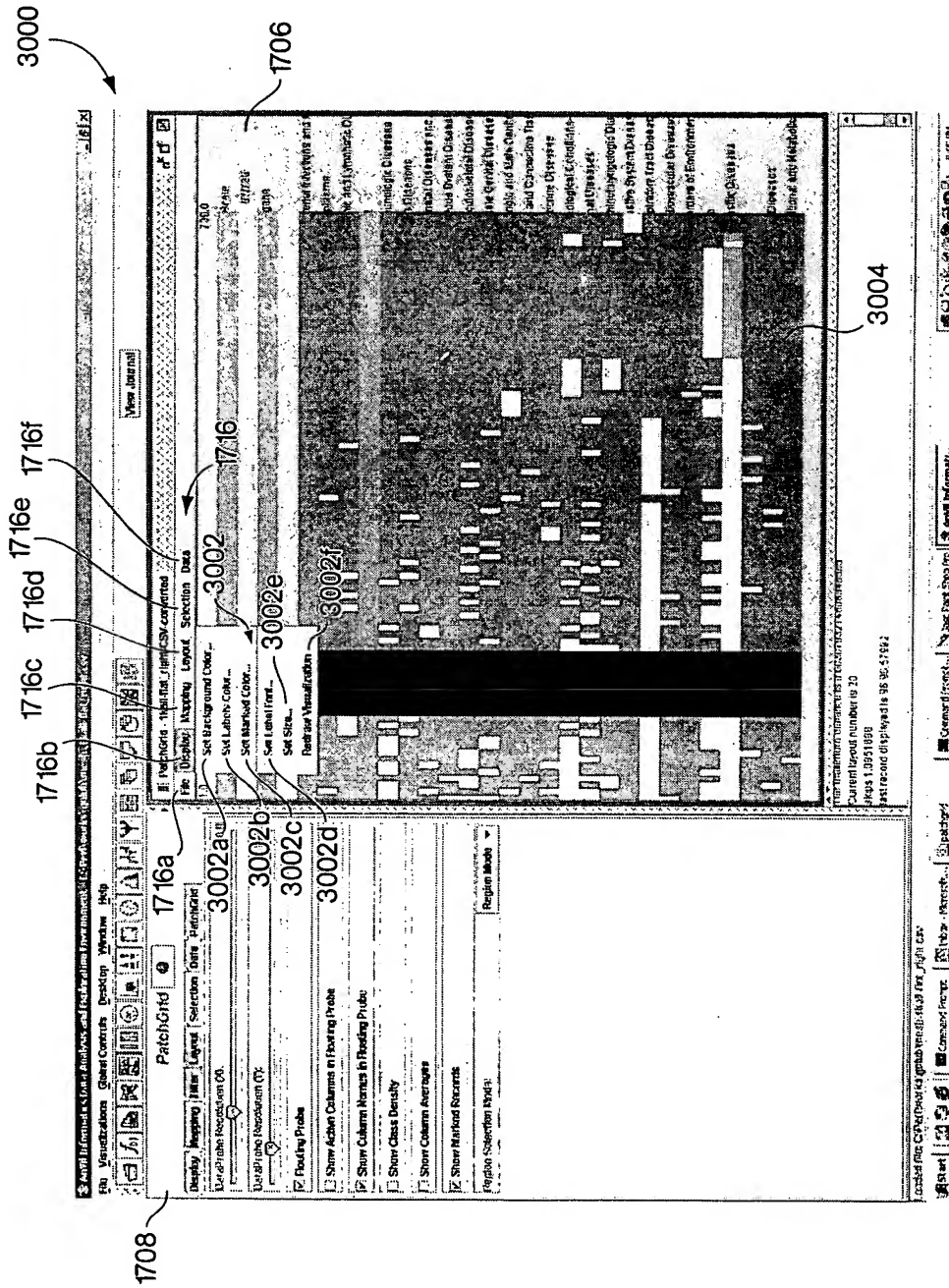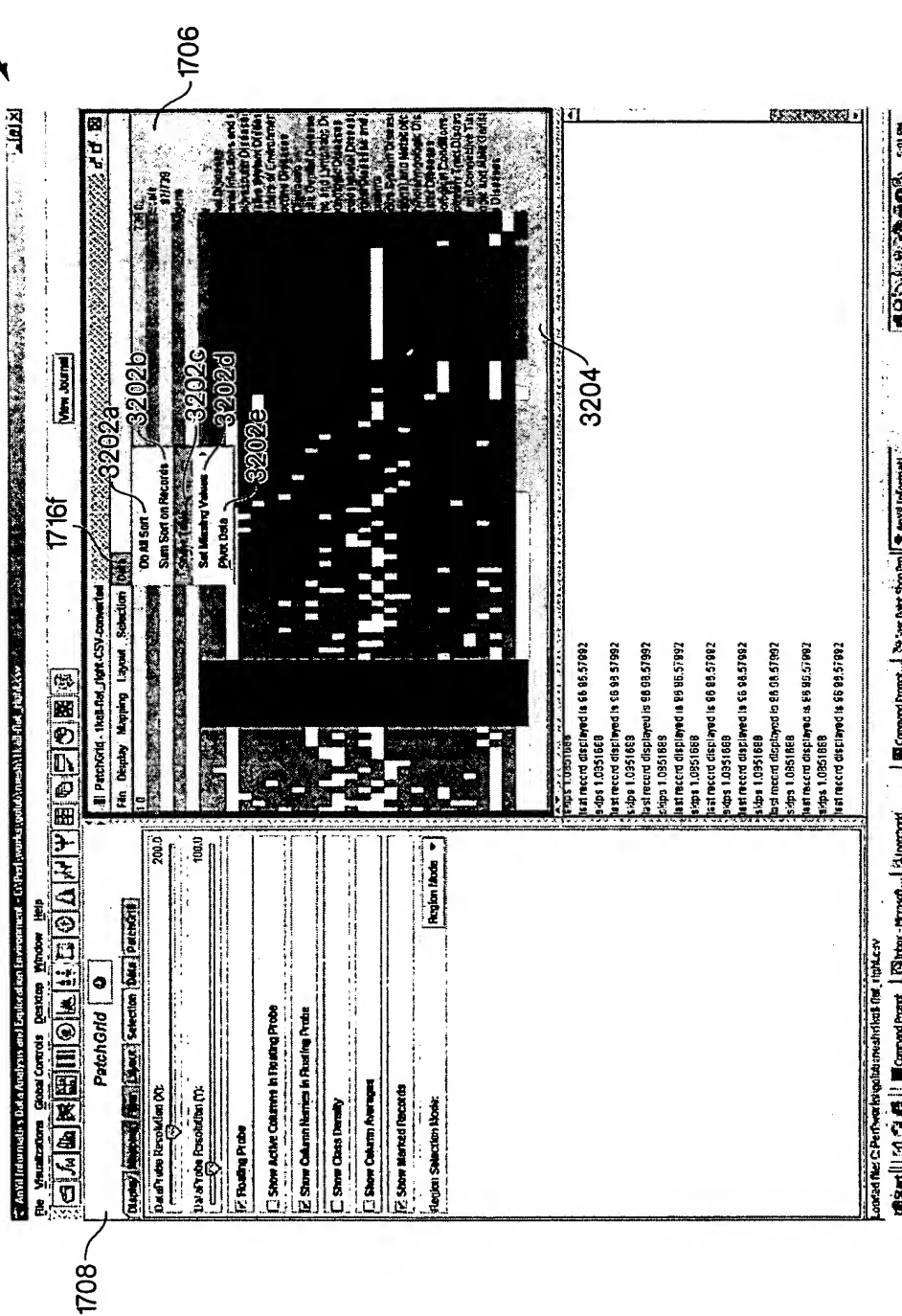
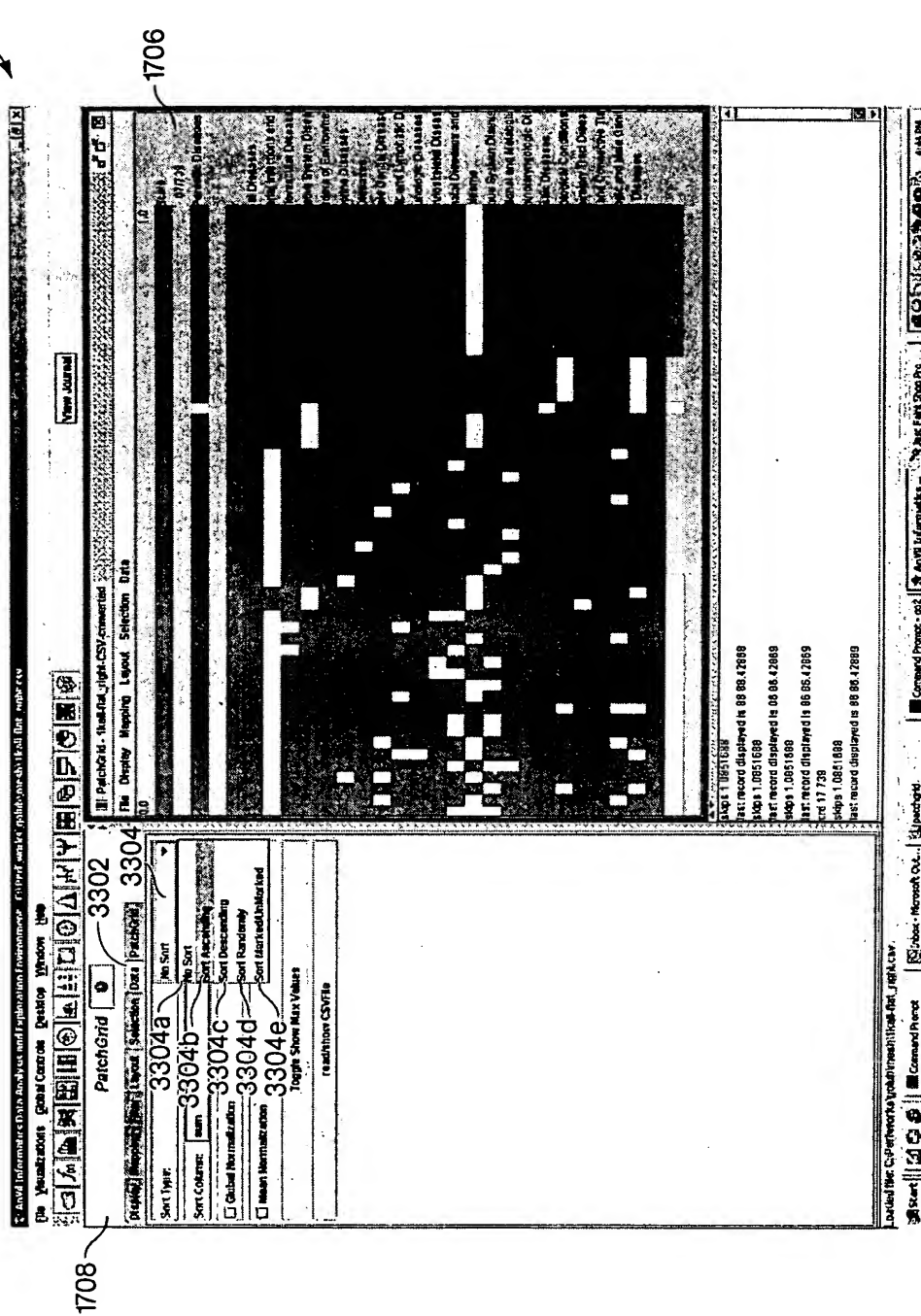3802 — fR3 fmla-CH2NO-

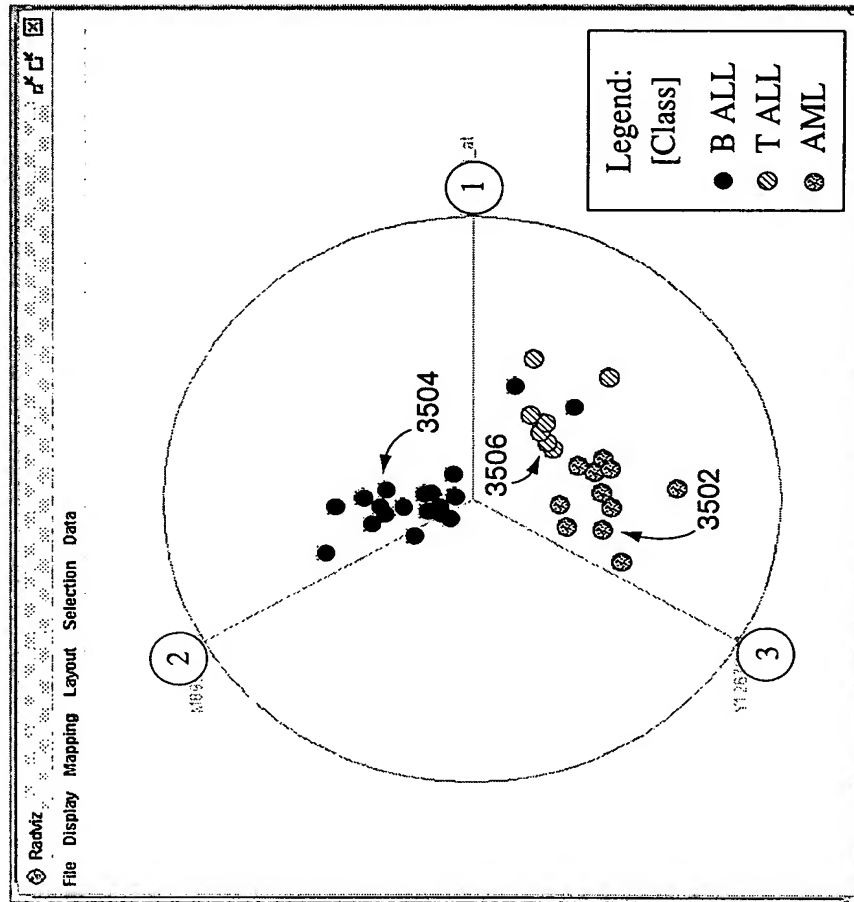fR3 fmla-C2H6N-

fR4 fmla-C7H13-

fR4 fmla-CH3-

fR4 fmla-H-

fR4 fmla-C5H11-

fR4 fmla-C4H9-

fR4 fmla-H-

fR3 fmla-Cl-

fR3 fmla-I-

fR3 fmla-CN-

fR3 fmla-Dr-

3804 — fR3 fmla-NO2-

fR3 fmla-F-

3806 3808

Color Legend:
Half Rainbow
Selectivity
■ Inactive
□ Active

Record	LC/MS	Assay 1	Assay 2	Kd 1	Kd 2	R1	R2	R3	R4	R5	Select
937	pass	0.087	355.5	591.7	9.51	C5H5-	C6H1 1-	CN-	C4H9-	3.00	good
937	pass	0.01	456.4	0.87	0.11	CH3-	C6H1 1-	CN-	C4H9-	4.43	good
937	pass	0.007	358.8	44.7	3.89	H-	C6H5-	CN-	C4H9-	5.58	good
937	pass	0.002	495.8	78.35	57.52	C9H8N-	C6H1 1-	CN-	C4H9-	6.44	good

3810

Fig. 40

Fig. 41

Record	LC/MS	Assay 1	Assay 2	Kd 1	Kd 2	R1	R2	R3	R4	S5	Select
937	pass	0.087	355.5	591.7	9.51	C5H5-	C6H1 1-	CN-	C4H9-	3.00	good
951	pass	0.01	456.4	0.87	0.11	CH3-	C6H1 1-	CN-	C4H9-	4.43	good
953	pass	0.007	358.8	44.7	3.89	H-	C6H5-	CN-	C4H9-	5.58	good
956	pass	0.002	495.8	78.35	57.52	C9H8N-	C6H1 1-	CN-	C4H9-	6.44	good
958	pass	0.001	305.8	0.14	7.6	H-	C6H1 1-	CN-	C4H9-	7.08	good

Color Legend:
Half Rainbow
Selectivity
■ Inactive
□ Active

Method and System for Data Analysis
Serial No.: 10/077,694
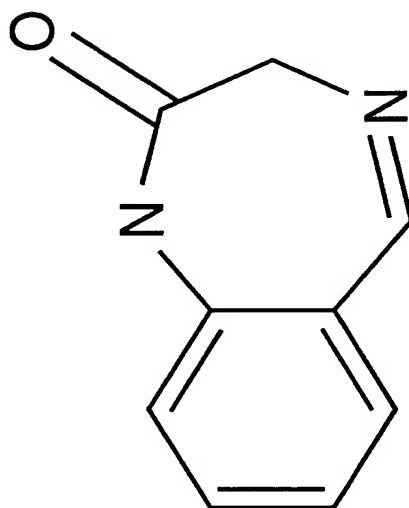Inventors: Grinstein, et al.
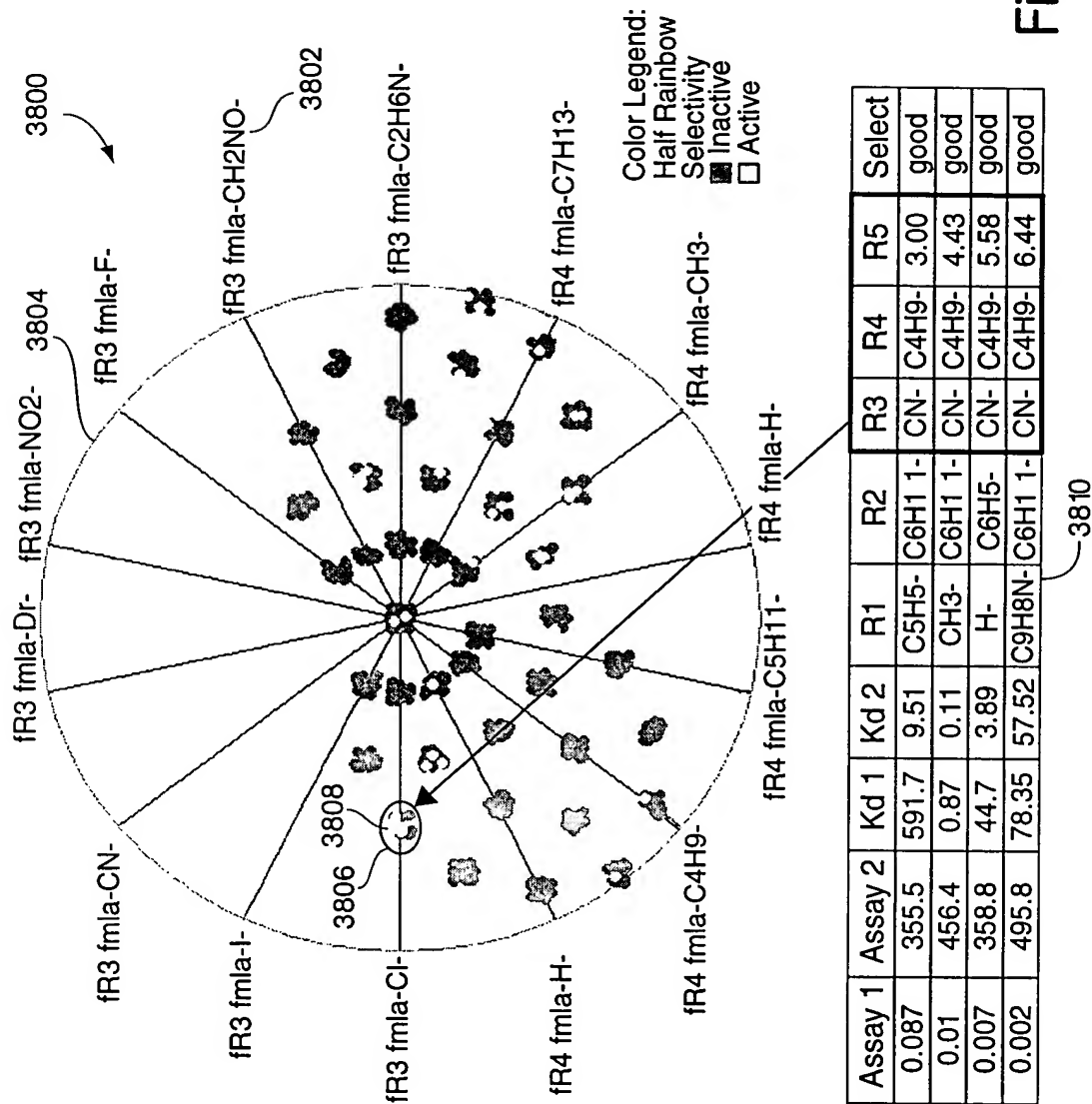Atty. Docket No.: ANVI-P01-001

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260 Descriptors

260 Descriptors

4200

4202

4204

4206

Fig. 42

Title: Method and System for Data Analysis
Serial No.: 10/077,694
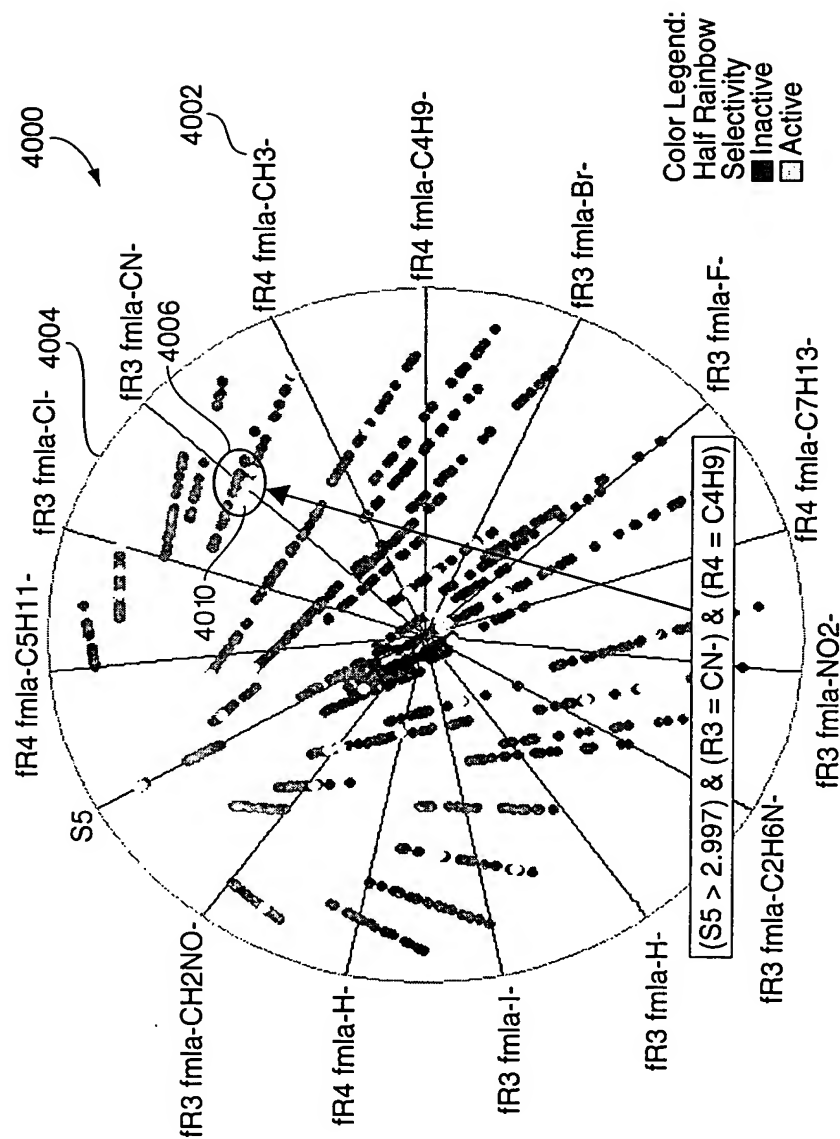Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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150 Chemical Classes

166 ISIS Keys

Shows ISIS Key Composition of each Chemical Class

4300

4302

4304

4306

Key off

Key on

Fig. 43

Title: Method and System for Data Analysis
Serial No.: 10/077,694
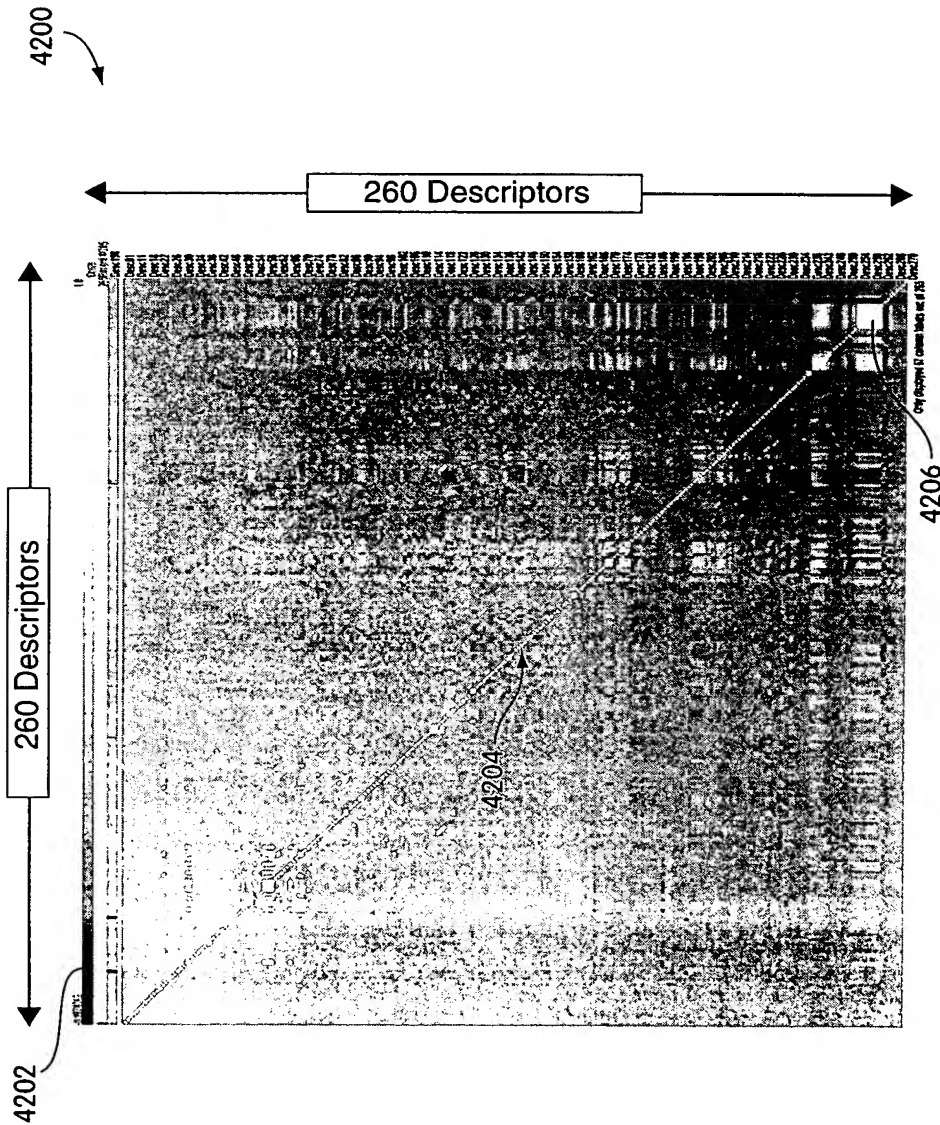Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 44

166 ISIS Keys

150 Chemical Classes

4300
4302
4308b
4308a

ISIS Keys Clustered to
show chemical classes
with similar keys

Key off
Key on

Method and System for Data Analysis
Serial No.: 10/077,694
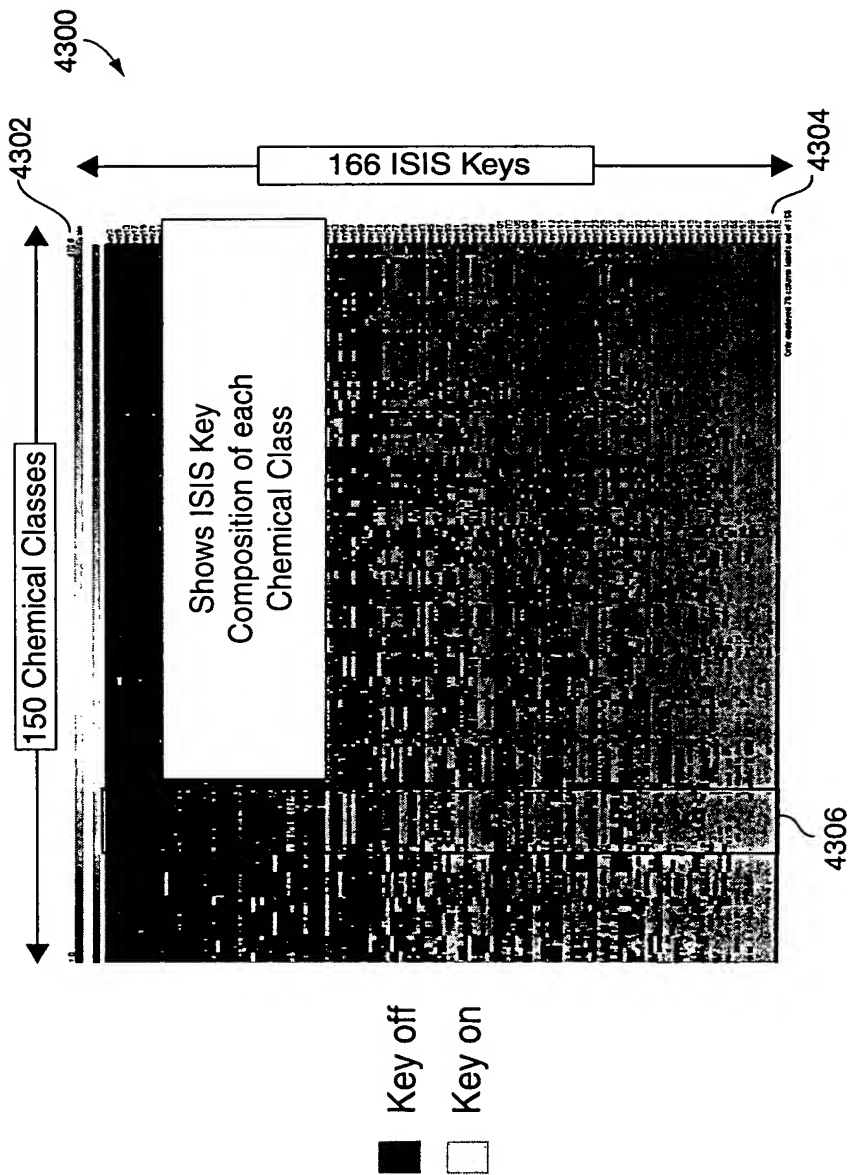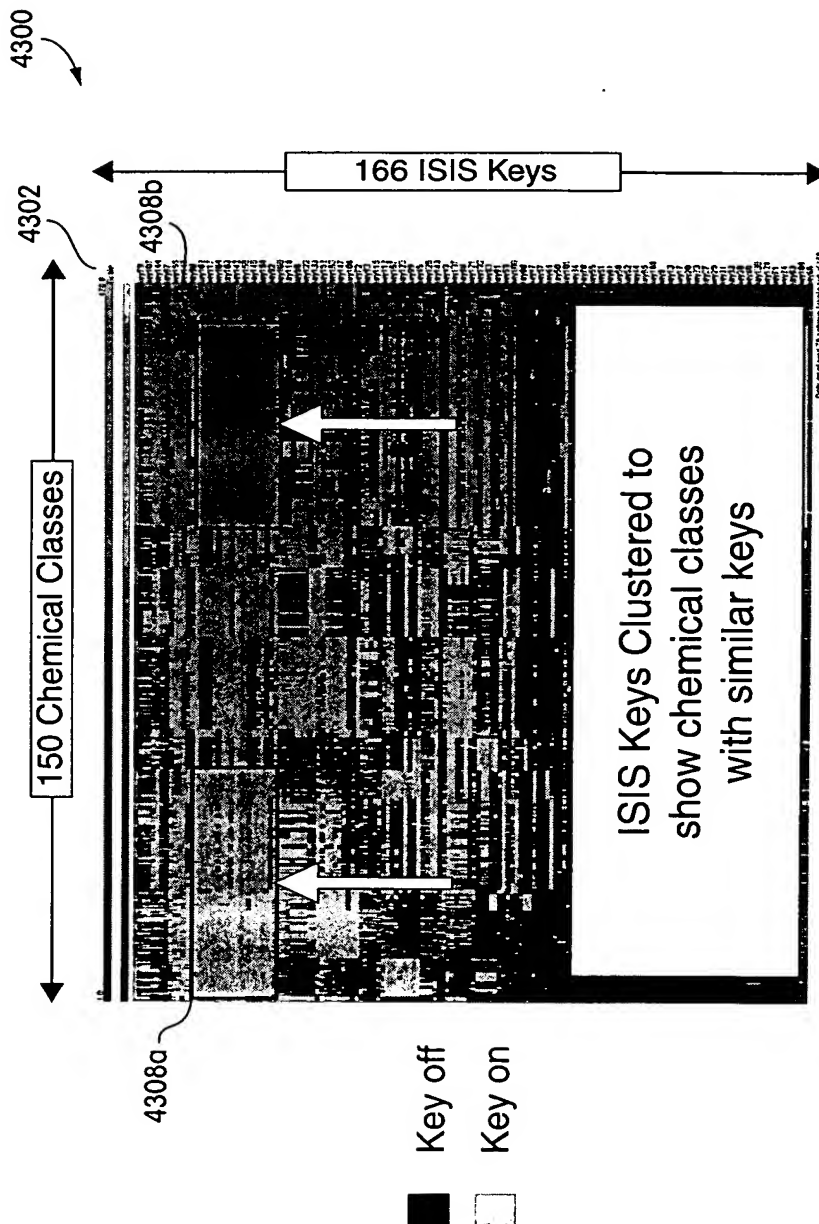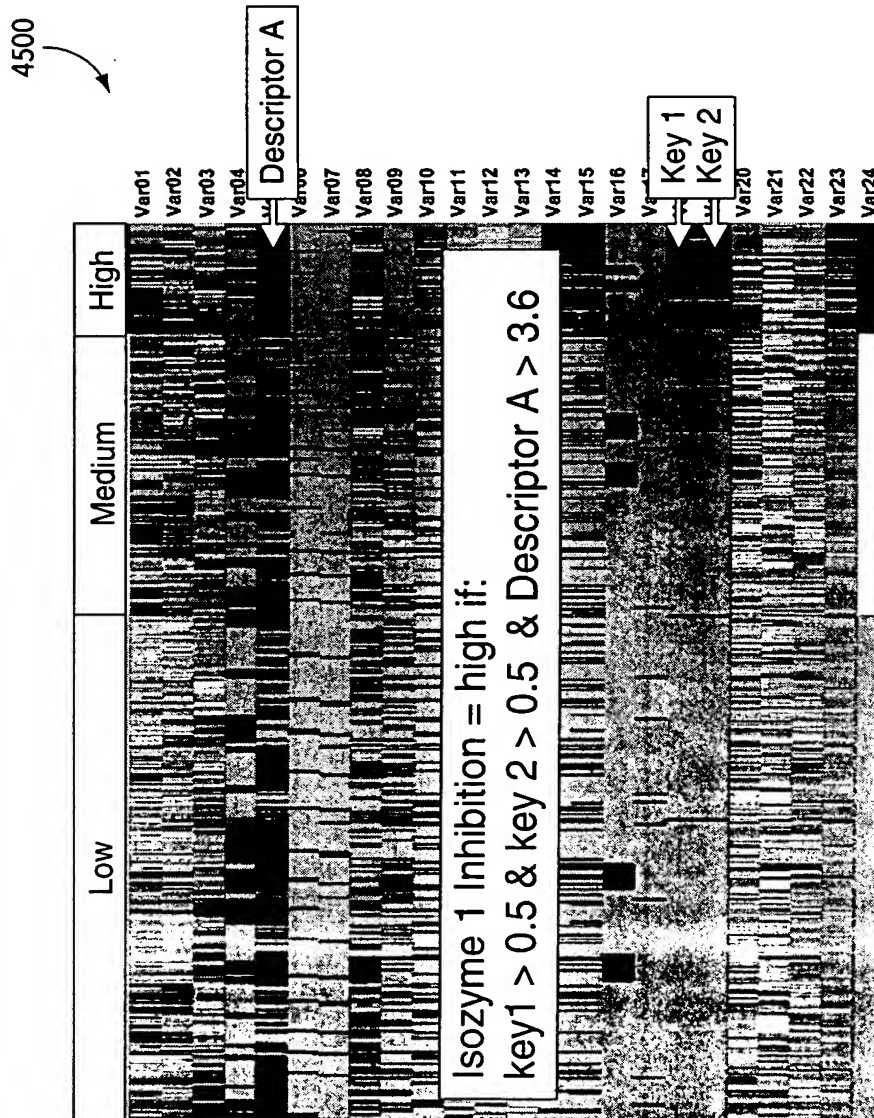Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 45

4500

Descriptor A

Key 1
Key 2

Var01 Var02 Var03 Var04 Var07 Var08 Var09 Var10 Var11 Var12 Var13 Var14 Var15 Var16 Var20 Var21 Var22 Var23 Var24

High
Medium
Low

Isozyme 1 Inhibition = high if:
key1 > 0.5 & key 2 > 0.5 & Descriptor A > 3.6

Method and System for Data Analysis
Serial No.: 10/077,694
Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 46

Method and System for Data Analysis
Serial No.: 10/077,694
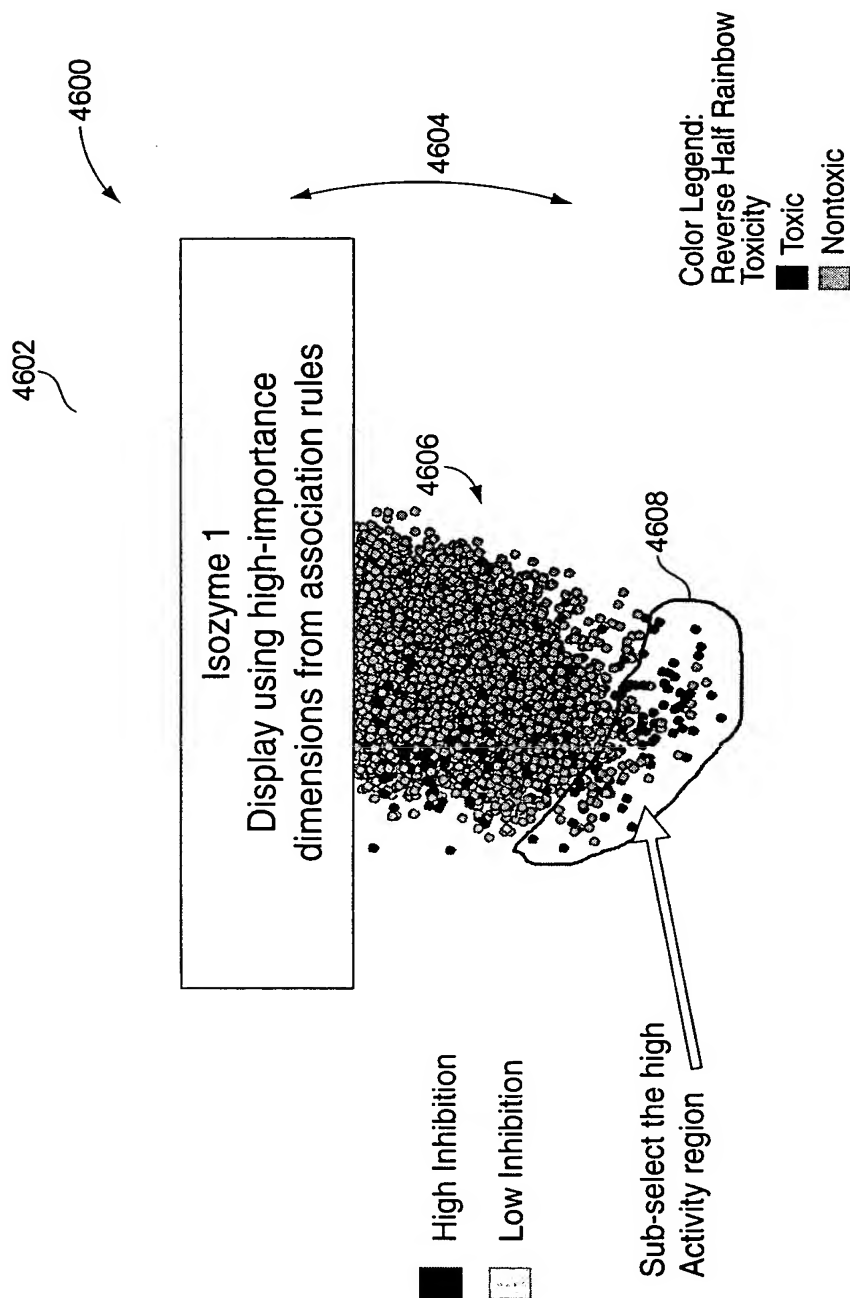Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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Fig. 47

: Method and System for Data Analysis
Serial No.: 10/077,694
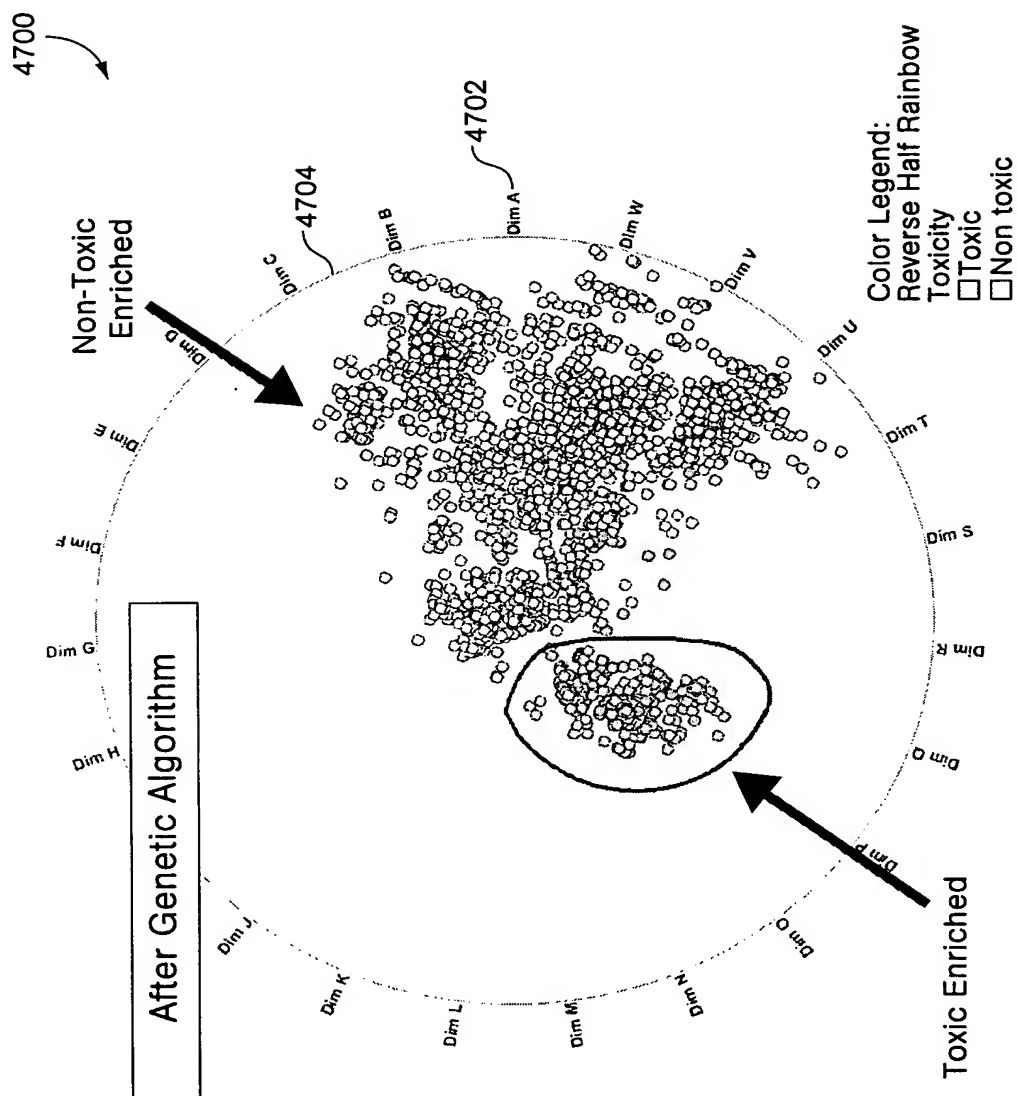Inventors: Grinstein, et al.
Atty. Docket No.: ANVI-P01-001

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After AP Algorithm

4802

Color Legend:
Half Rainbow
◉ Non-Toxic
● Toxic

4800

Fig. 48

e: Method and System for Data Analys
Serial No.: 10/077,694
Inventors: Grinstein, et al.
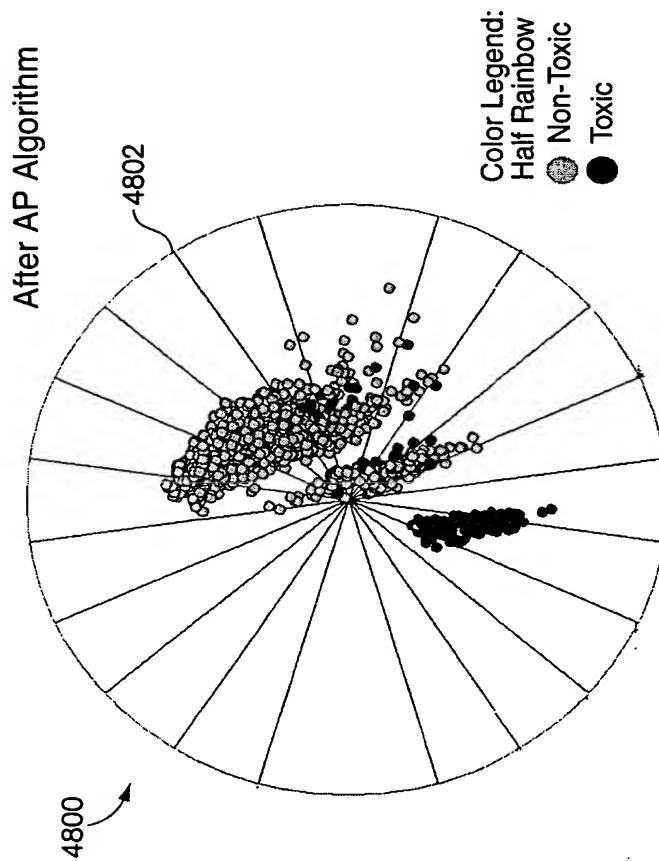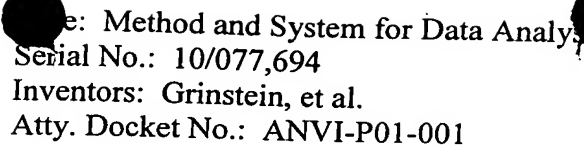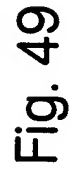Atty. Docket No.: ANVI-P01-001

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Fig. 49